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(54) Title: NOVEL BACE PROTEINS, NUCLEIC ACID MOLECULES THEREFOR, NOVEL CRYSTAL STRUCTURE OF NOVEL BACE PROTEINS, AND METHODS FOR MAKING AND USING

(57) Abstract: Disclosed and claimed are novel BACE proteins, crystal structures thereof, nucleic acid molecules therefor, and methods for making and using and uses of the same, especially for ascertaining inhibitors of BACE; and thus, disclosed and claimed too are inhibitors of BACE and methods of making and using the same.



5 TITLE OF THE INVENTION

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NOVEL BACE PROTEINS, NUCLEIC ACID MOLECULES THEREFOR, NOVEL CRYSTAL STRUCTURE OF NOVEL BACE PROTEINS, AND METHODS FOR MAKING AND USING FIELD OF THE INVENTION

This invention relates generally to structural studies of the soluble Beta-site APP cleaving enzyme (BACE) catalytic domain (e.g., the aspartyl protease domains of BACE) and the corresponding structural information obtained by X-ray crystallography.

Moreover, the present invention relates to any one or more of:

A catalytic domain of BACE, or a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or apo-BACE crystals which are BACE crystals with no ligand bound, regardless of the source of the BACE) and/or apo-BACE crystals which are capable of being soaked with ligand to give complexes and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a=236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, b= 105.02\AA or $105.02\text{\AA} \pm \text{standard deviation}$ (0.2Å) or $105.02\text{\AA} \pm \text{cell variability}$ of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° ± standard deviation (0.2°) between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing;

Apo-BACE crystals that can be soaked, e.g., with ligands such as inhibitory or modulatory ligands, to give complexes, such as protein-ligand complexes;

A crystalline form of BACE or a BACE that has an active site containing one or more ligands other than the natural substrate or the substrate that occurs naturally or physiologically within the active site or apo-BACE crystals with no ligand bound, regardless of the source of the BACE; for instance, for use in rational drug design, as well as methods for ligand screening and design by X-ray crystallography;

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BACE proteins comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure (included in the term "BACE proteins") - such as those, when compared with other BACE proteins (such as Genbank accession P56817) have one or more of: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453) - whereby such proteins can also optionally include one or more of: a tag such as a His tag (e.g., a HIS6 tag) for instance to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence; and a tag such as a FLAG tag to allow differentiation of species arising from incomplete pro-peptide cleavage (and separation if required);

BACE proteins that have one or more mutations to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals, such as with reference to Genbank accession P56817: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453);

BACE proteins that include one or more of: a tag such as a His tag (e.g., a HIS₆ tag) for instance to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of

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the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence; and a tag such as a FLAG tag to allow differentiation of species arising from incomplete pro-peptide cleavage (and separation if required);

One or more nucleic acid molecules (e.g., an isolated nucleic acid molecule) encoding the BACE proteins or at least a functional portion thereof including any of the foregoing proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure including those having reduced GC content via silent mutations from nucleotide sequences derived from wild-type BACE that would also encode the foregoing;

Vectors or cells (e.g., viral vectors such as baculovirus, bacterial vectors such as *E. coli*, mammalian cells such as CHO cells, or DNA plasmids) containing and/or expressing any one or more of the nucleic acid molecules and/or BACE proteins – the latter can include prior BACE proteins especially when there is co-expression thereof with a gene product - an enhancer - that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme, for instance a convertase or a transcription enhancer or a translation enhancer or both a transcription and translation enhancer, for instance a prohormone convertase such as the prohormone convertase furin especially when the vector or cell system is baculovirus and/or insect cells, and thus also vectors or cells containing and/or expressing the nucleic acid molecules and/or BACE proteins and a nucleic acid molecule encoding the enhancer as well as kits containing separately packaged isolated nucleic acid molecules comprising (i) a BACE-protein encoding nucleic acid molecule and (ii) a nucleic acid molecule encoding the enhancer, for use in vectors or cells for the co-expression thereof;

Expression through or by vectors or cells of that which is encoded by the nucleic acid molecules and/or contained in the aforementioned vectors or cells and/or of the gene products and/or the amino acid sequences and/or the BACE proteins, including co-expression thereof, or of other nucleic acid molecules encoding BACE proteins, with a gene product that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme, e.g., a convertase, for instance a prohormone convertase such

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as the prohormone convertase furin especially when the vector or cell system is baculovirus and/or insect cells;

Methods for crystallizing BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain;

Methods for determining the crystal structure of BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain;

Uses of that which is encoded by the nucleic acid molecules and/or the gene products and/or the amino acid sequences and/or the BACE proteins, for instance in screening assays such as drug or patient screening assays or in generating products therefor (such as for generating antibodies to the catalytic domain and/or to BACE proteins which are useful in such assays), as well as such assays and products therefor, and uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells, for preparing such uses or assays and/or components for such uses or assays;

Products from such assays ("assay products"), as well as uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells for preparing such assay products and/or components for such assay products;

Inhibitors or modulators of BACE and/or inhibitors or modulators of the production of A β or fragments thereof, for instance, such inhibitors or modulators as determined through the assays of the present invention and/or through contact with and binding to or otherwise inhibiting or modulating BACE proteins of the present invention, such as a compound or composition which binds to and/or inhibits and/or modulates and/or interacts with a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or having an unoccupied or substantially unoccupied active site and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 105.02Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° \pm standard deviation (0.2Å) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of

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BACE (e.g., from growth in the presence of OM99-2) or cell dimensions $a=238.3\text{\AA}$ or $238.3\text{\AA}\pm$ standard deviation (0.2Å) or $238.3\text{\AA}\pm$ cell variability of 3\AA , $b=107.4\text{\AA}\pm$ standard deviation (0.2Å) or $107.4\text{\AA}\pm$ cell variability of 3\AA , and $c=60.4\text{\AA}$ or $60.4\text{\AA}\pm$ standard deviation (0.2Å) or $60.4\text{\AA}\pm$ cell variability of 3\AA and $\beta=101.89^{\circ}$ or $101.89^{\circ}\pm$ standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing (excluding, of course, prior known inhibitors, modulators, if any, of BACE and/or inhibitors, modulators of the production of AB or fragments thereof);

Uses of such assay products and/or inhibitors and/or modulators, for instance in treating maladies, conditions, diseases and the like such as Alzheimer's disease (AD) involving BACE activity and/or Aβ or fragments thereof and/or in formulating medicaments for such treatments, as well as of uses of the nucleic acid molecules, vectors or cells, the methods and/or the aforementioned expression via vectors or cells, for such treatment and/or a component thereof and/or for preparing such medicaments and/or a component thereof, such that methods for preparing such medicaments including use of any of the foregoing is included, *inter alia*.

And a data storage medium encoded with the structural co-ordinates of crystallized BACE or at least a functional portion thereof. Such data storage material is capable of displaying such structures, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure co-ordinates to solve the structure of similar or homologous proteins or protein complexes. In addition, this invention relates to methods of using structure co-ordinates to screen and design compounds, including inhibitory compounds, that bind to BACE or homologues thereof. The present invention also relates to compositions and crystals of BACE in complex with a BACE inhibitor. *Cf.* WO 01/37194.

Various documents are cited in this text. Citations in the text can be by way of a citation to a document in the reference list, e.g., by way of author(s) and document year citation to a document listed in the reference list, or by full citation in the text to a document that may or may not also be listed in the reference list.

There is no admission that any of the various documents cited in this text are prior art as to the present invention. Any document having as an author or inventor person or persons named as an inventor herein is a document that is not by another as to the inventive entity herein.

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All documents cited in this text ("herein cited documents") and all documents cited or referenced in herein cited documents are hereby incorporated herein by reference. Likewise, teachings of herein cited documents and documents cited in herein cited documents can be employed in the practice and utilities of the present invention.

BACKGROUND OF THE INVENTION

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Alzheimer's disease (AD) is estimated to afflict more than 20 million people worldwide and is believed to be the most common form of dementia (Newsday (New York), Friday, July 6, 2001, City Edition, page A24). AD is a progressive dementia characterized by amyloid plaques and intracellular neurofibrillary tangles that accumulate in the brain and are thought to be responsible for the mental decline in Alzheimer's patients.

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Beta-amyloid protein $(A\beta)$ is the major constituent of the amyloid plaques, which are characteristic of AD (De Strooper and Konig, 1999).

A β is a 39-42 amino acid residue peptide formed by the specific cleavage of a class I transmembrane protein called the amyloid precursor protein (APP) by two proteases, β - and γ -secretase (the A β fragment).

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 β -secretase cleaves APP between residues Met671 and Asp672 (numbering corresponds to the 770 amino acid isoform of APP) to form the N-terminus of A β . A second cleavage of the peptide is associated with γ -secretase to form the C-terminus of the A β peptide. β and γ -secretases cleave the amino and carboxy terminal ends of the A β domain, respectively. A third enzyme, α -secretase, has recently been identified which cleaves APP within the A β domain between residues 16 and 17 of the A β fragment (Howlett et al., 2000).

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The therapeutic potential of inhibiting and/or modulating the deposition of Aβ has motivated many groups to isolate and characterize secretase enzymes and to identify their potential inhibitors (*see*, *e.g.*, WO01/23533 A2, EP0855444A2,WO00/17369, WO00/58479, WO00/47618, WO01/00665; WO01/00663; U.S. Patent No. 6,245,884 (Hook), U.S. Patent No. 6,221,667 (Reiner et al.), U.S. Patent No. 6,211,235 (Wu et al.)). Indeed, it also has been reported in the popular press that "[d]rug makers are studying medicines called gamma-secretase inhibitors, which aim to block the cleavage process" (Newsday (New York), Friday, July 6, 2001, City Edition, page A24).

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Consequently, a number of potential candidates for these enzymes have recently been reported in the literature: Several groups have identified and isolated aspartate proteases that have

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β-secretase activity (Hussain et al., 1999; Lin et. al, 2000; Yan et. al, 1999; Sinha et. al., 1999 and Vassar et. al., 1999). β-secretase is also known in the literature as Asp2 (Yan et. al, 1999), Beta site APP Cleaving Enzyme (BACE) (Vassar et. al., 1999) or memapsin-2 (Lin et al., 2000).

BACE was identified using a number of experimental approaches such as EST database analysis (Hussain et al. 1999); expression cloning (Vassar et al. 1999); identification of human homologs from public databases of predicted *C. elegans* proteins (Yan et al. 1999) and finally utilizing an inhibitor to purify the protein from human brain (Sinha et al. 1999). Thus, five groups employing three different experimental approaches has led to the identification of the same enzyme, making a strong case that BACE is a β-secretase. Mention is also made of the patent literature: WO91/13904, EP518955, EP732399, WO92/03542, WO92/07068, WO96/40885, EP87/1720, U.S. Patents Nos. 5,942,400 and 5,744,346, EP855444, EP1037977, WO00/17369, WO01/23533, WO0047618, WO00/58479, WO01/00663, WO01/00665, EP848062, U.S. Patents Nos. 6,025,180 and 6,162,639, EP1047788 and WO99/33963, WO99/46281, WO98/11236, U.S. Patent No. 5,942,400 and WO94/13319.

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Indeed, BACE is a membrane bound protein which is synthesized as a partially active proenzyme, and is most abundantly expressed in brain tissue. It is thought to represent the major β -secretase activity.

BACE activity may be considered to be a rate-limiting step in the production of Aβ. This makes BACE of special interest in the pathology of Alzheimer's disease and other maladies that involve Aβ, or fragments thereof (e.g., amyloid plaques and amyloid angiopathy also characterize the brains of individuals with Trisomy 21 or Down's Syndrome, Hereditary Cerebral Hemorrhage with Amyloidosis of the Dutch Type (HCHWA-D), *inter alia*; *see also* U.S. Patent No. 6,211,235), and therefore an important candidate for the development of drugs as a treatment against Alzheimer's disease and/or against such other maladies.

Furthermore, as reported in the popular press, Newsday (New York), Friday, July 6, 2001, City Edition, page A24, that day's edition of Science includes *in vitro* findings by investigator Thomas Sudhof of the Howard Hughes Medical Institute which suggest that gamma secretase may be implicated in another function, but that it is not known if those findings apply to humans or which genes may be involved. Nonetheless, inhibiting gamma secretase may have issues which are addressed by the present invention involving inhibiting BACE the production of $A\beta$ or fragments thereof.

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The likelihood of developing Alzheimer's disease increases with age, and as the aging population of the world increases, this disease may become a greater and greater problem. In addition, there is a familial link to AD and consequently any individuals possessing the double mutation of APP known as the Swedish mutation (in which the mutated APP forms a considerably improved substrate for BACE) have a much greater chance of developing AD and also of

developing it at an early age (see also U.S. Patent No. 6,245,964 pertaining to transgenic rodent comprising APP-Swedish).

It would therefore be useful to inhibit and/or modulate the deposition of $A\beta$ and portions thereof; for instance by inhibiting and/or modulating BACE proteins through inhibitors or modulators thereof ascertained from BACE proteins having a particular crystal structure or having a structure as herein set forth.

Hence, drugs that reduce or block BACE activity would reduce $A\beta$ levels and levels of fragments of $A\beta$ in the brain or elsewhere where $A\beta$ or fragments thereof deposit and thus slow the formation of amyloid plaques and the progression of AD or other maladies involving deposition of $A\beta$ or fragments thereof (Yankner, 1996; De Strooper and Konig, 1999).

Further, reaction systems comprising Beta secretase have been asserted to be useful in screening assays, e.g., to identify inhibitors or modulators and antibodies raised against Beta-secretase have been asserted to be useful for screening and other assays; see, e.g., U.S. Patent No. 6,221,645 and other documents cited herein; and thus, the present invention is likewise useful in such assays in generating antibodies.

There has been the production of certain active recombinant BACEs - different from those of the herein invention - using heterologous expression systems for mammalian cells (Vassar et al, 1999, Hassain et al, 1999), insect cells (Mallender et al, 2001) and bacterial cells (Lin et al 2000). While the production of these BACEs shows that no undue experimentation is needed to practice the present invention, these prior systems had deficiencies addressed by the herein invention.

Indeed, prior to the present invention there was a need to produce a soluble recombinant BACE protein with an improved crystal structure that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or having an unoccupied or substantially unoccupied active site and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å ± standard

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deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or 105.02Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2), as well as amino acid sequences therefor, nucleic acid molecules encoding them, and other aspects of the present invention as herein discussed.

In addition, the study of crystal structure and symmetry is developed (*See, e.g.*, Cotton and Wilkinson, Inorganic Chemistry (John Wiley & Sons, Fourth Ed. 1980), especially Ch. 2). X-ray crystallography, or more generally crystallography, is an established, well-studied technique that provides what can best be described as a three-dimensional picture of what a molecule looks like in a crystal, and is useful for determining whether a compound that is not a known ligand of a target biomolecule can indeed bind as a ligand to a target biomolecule (*see, e.g.*, WO 99/45379; U.S. Patent No. 6,087,478; U.S. Patent No. 6,110,672); and, there are additional techniques for identifying drug cores (*see, e.g.*, WO 98/57155 regarding fragment-based screening). Mention is also made of U.S. Patents Nos. 6,128,582, 6,153,579, 6,077,682, and 6,037,117 and PCT publications WO01/37194 and WO00/47763 for additional information on aspects of structure-based drug design and homology modelling.

These techniques can be employed with the herein disclosed BACE crystals and proteins, especially those that are without any ligands typically found in wild-type BACE, to rationally design compounds that inhibit or modulate, e.g., bind to or interact with BACE; and, the use of these techniques, in combination with herein disclosed BACE crystals and proteins it is believed has not been heretofore taught or suggested in the art.

OBJECTS AND SUMMARY OF THE INVENTION

Without excluding inventions otherwise herein disclosed, the present invention can provide one or more of the following embodiments.

The present invention in an embodiment provides a catalytic domain of BACE, such as a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates

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the need for refolding and/or a BACE protein having an unoccupied or substantially unoccupied active site (apo-BACE crystals with no ligand bound, regardless of the source of the BACE) and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3\AA , b= 105.02\AA or $105.02\text{Å} \pm$ standard deviation (0.2Å) or $105.02\text{Å} \pm$ cell variability of 3\AA , and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° ± standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å or 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or $60.4\text{\AA} \pm \text{standard deviation}$ (0.2Å) or $60.4\text{\AA} \pm \text{cell variability of 3Å}$ and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P2₁ form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand.

The present invention likewise provides apo-BACE crystals that can be soaked, e.g., with ligands such as inhibitory or modulatory ligands, to give complexes, such as protein-ligand complexes.

The present invention in another embodiment provides a crystalline form of BACE or a BACE that has an active site containing one or more ligands other than the natural substrate or the substrate that occurs naturally or physiologically within the active site or apo-BACE crystals with no ligand bound, regardless of the source of the BACE; for instance, for use in rational drug design, as well as methods for ligand screening and design by X-ray crystallography.

In regard to this, the invention further provides a method for ligand screening and/or design, e.g., by X-ray crystallography and/or nuclear magnetic resonance (NMR). The method can include exposing the apo crystals or BACE crystals with no ligand bound (i.e., with an unoccupied active site, regardless of the source of the BACE) to one or more test samples, and determining whether a ligand-BACE complex is formed, e.g., obtaining an X-ray crystal diffraction pattern to

determine whether a ligand-BACE complex is formed or using NMR to determine whether such a complex is formed. The BACE can be exposed to the test samples by either co-crystallizing the BACE in the presence of the one or more test samples or soaking the BACE in a solution of one or more test samples. Structural information from ligand-BACE complexes can be used to design ligands that bind tighter, that bind more specifically, that have better biological activity or have a better safety profile. Cf. WO99/45379.

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The present invention thus further provides a computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the atoms in the BACE catalytic domain, e.g., BACE protein as herein provided and/or such information with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system: (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally complementary to said data set; (d) optionally constructing, using computer methods, a model of a chemical structure having a portion that is structurally complementary to said data set and (e) outputting to said output device the selected chemical structures having a portion complementary to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits or modulates or interacts with BACE. Cf. U.S. Patent No. 5,835,382.

In this way, one can rationally identify and/or design inhibitors or modulators of BACE or compounds that interact with BACE. And, in this regard, mention is made that the skilled artisan can employ the products found in the wild-type BACE catalytic domain as a portion of the information to be inputted or employed in the rational design and/or identification of inhibitors or modulators of BACE or compounds that interact with BACE. Furthermore, an inhibitor of BACE can be competitive, non-competitive, uncompetitive, or irreversible; and, inhibitors of BACE are of significant technical and commercial interest.

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The present invention also provides BACE proteins comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure (included in the term "BACE proteins") - such as those, when compared with other BACE proteins (such as Genbank accession P56817) have one or more of: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at an 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453) - whereby such proteins can also optionally include one or more of: a tag such as a His tag (e.g., a HIS₆ tag) for instance to facilitate purification (cf. U.S. Patent No. 6,020,143); a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence (cf. U.S. Patents Nos. 6,245,532, 5,516,657); and a tag such as a HA or FLAG tag to allow differentiation of species arising from incomplete pro-peptide cleavage (and separation if required) (cf. U.S. Patents Nos. 6,190,874, 6,083,732).

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The present invention thus further provides BACE proteins that have one or more mutations to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals, such as with reference to Genbank accession P56817: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as

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asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453).

Advantageously, the BACE protein has all four of the mutations and the truncation.

The present invention additionally provides BACE proteins that include one or more of: a tag such as a His tag (e.g., a HIS₆ tag) for instance to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence; and a tag such as a FLAG tag to allow differentiation of species arising from incomplete pro-peptide cleavage (and separation if required).

Even further still, the present invention provides one or more nucleic acid molecules (e.g., an isolated nucleic acid molecule) encoding the BACE proteins or at least a functional portion thereof including any of the foregoing proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure including those having reduced GC content via silent mutations from nucleotide sequences derived from wild-type BACE that would also encode the foregoing.

In yet further embodiments, the present invention provides vectors or cells (e.g., viral vectors such as baculovirus, bacterial vectors such as *E. coli*, mammalian cells such as CHO cells, or DNA plasmids) containing and/or expressing any one or more of the nucleic acid molecules and/or BACE proteins – the latter can include prior BACE proteins especially when there is coexpression thereof with a gene product - an enhancer - that enhances in the particular vector or cell system, the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme e.g., a convertase, or a transcription enhancer or a translation enhancer or both a transcription and translation enhancer (*cf.*. U.S. Patents Nos. 6,130,066, 6,004,777, 5,990,091), for instance a prohormone convertase such as the prohormone convertase furin (*cf.* Laprise et al. 1998) when the vector or cell system is baculovirus and/or insect cells, and thus also vectors or cells containing and/or expressing the nucleic acid molecules and/or BACE proteins and a nucleic acid molecule encoding the enhancer as well as kits containing separately packaged isolated nucleic acid molecules for such co-expression, e.g., a kit containing separately packaged nucleic acid molecules

comprising (i) a BACE-protein encoding nucleic acid molecule and (ii) a nucleic acid molecule encoding the enhancer, for use in vectors or cells for the co-expression thereof;

The invention thus also provides expression through or by vectors or cells of that which is encoded by the nucleic acid molecules and/or contained in the aforementioned vectors or cells and/or of the gene products and/or the amino acid sequences and/or the BACE proteins, including co-expression thereof, or of other nucleic acid molecules encoding BACE proteins, with a gene product that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme, e.g., a convertase, for instance a prohormone convertase such as the prohormone convertase furin especially when the vector or cell system is baculovirus and/or insect cells.

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As the invention involves a unique crystal structure of BACE, the invention provides methods for crystallizing BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain.

Similarly, the invention provides methods for determining the crystal structure of BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain.

The invention further contemplates uses of that which is encoded by the nucleic acid molecules and/or the gene products and/or the amino acid sequences and/or the BACE proteins, for instance in screening assays such as drug or patient screening assays or in generating products therefor (such as for generating antibodies to the catalytic domain and/or to BACE proteins which are useful in such assays), as well as such assays and products therefor, and uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells, for preparing such uses or assays and/or components for such uses or assays.

Included within the ambit of the present invention are products from such assays ("assay products"), as well as uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells for preparing such assay products and/or components for such assay products.

The BACE protein of the present invention may be employed in screening for compounds which inhibit or modulate or activate or interact with this protein. Such compounds may be identified from cells or cell fractions, mixtures of natural products or chemical libraries.

The assay may comprise mixing the BACE polypeptide of the invention with a candidate compound in solution and measuring BACE activity in the mixture. It may also be advantageous to measure binding of the compound to the BACE polypeptide (or competition with binding of a known inhibitor) instead of an effect on enzyme activity. Alternatively, versions of the BACE protein containing the transmembrane region may be expressed in cells, and these cells (or membranes prepared from these cells) may be incubated with candidate compounds. The effect on BACE activity may then be assessed by measurement of cleavage of a suitable substrate, either added to the mixture or co-expressed in the cells.

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The protein or antibodies to the protein may also be used to identify receptors, through standard techniques. These include, but are not limited to, ligand binding or cross-linking assays in which the BACE protein is labeled and contacted with a source of the putative receptor, and biophysical techniques such as surface plasmon resonance.

The present invention even further contemplates inhibitors or modulators of BACE or compounds or compositions that interact with BACE and/or inhibitors or modulators of the production of AB or fragments thereof, for instance, such inhibitors as determined through the assays of the present invention and/or through contact with and binding to or otherwise interacting with, inhibiting or modulating BACE proteins of the present invention, such as a compound or composition or ligand which binds to and/or inhibits and/or interacts with and/or modulates a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or having an unoccupied or substantially unoccupied active site and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3\AA , b= 105.02\AA or 105.02\AA ± standard deviation (0.2Å) or 105.02\AA ± cell variability of 3\AA , and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° ± standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= $107.4\text{\AA} \pm \text{standard deviation}$ (0.2Å) or $107.4\text{\AA} \pm \text{cell variability of } 3\text{\AA}$ and $c = 60.4\text{\AA}$ or $60.4\text{\AA} \pm 60.4\text{\AA}$ standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2)

and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing (excluding, of course, prior known inhibitors and modulators of BACE and/or inhibitors or modulators of the production of $A\beta$ or fragments thereof).

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And, the present invention provides uses of such assay products and/or inhibitors and/or modulators and/or ligands, and/or compositions or compounds that interact with BACE, for instance in treating maladies, conditions, diseases and the like such as Alzheimer's disease (AD) involving BACE activity and/or $A\beta$ or fragments thereof and/or in formulating medicaments for such treatments, as well as of uses of the nucleic acid molecules, vectors or cells, the methods and/or the aforementioned expression via vectors or cells, for such treatment and/or a component thereof and/or for preparing such medicaments and/or a component thereof, such that methods for preparing such medicaments including use of any of the foregoing is included.

In a further embodiment, the present invention provides a Beta-site APP cleaving enzyme which comprises an amino acid sequence of SEQ ID NO: 5; advantageously, the amino acid sequence comprises a catalytic domain, and wherein the enzyme is in a crystalline form, such as herein defined.

In another embodiment the recombinant Beta-site APP cleaving enzyme comprises an amino acid sequence of SEQ ID NO: 5 (Figs. 1B, 2A, 8), as well as nucleic acid molecules encoding such an enzyme; for instance, a nucleic acid molecule comprising a sequence of SEQ ID NO: 4 or 10 (Figs. 1A, 2B, 7).

More in particular, with respect to the herein mentioned nucleic acid molecules and polypeptides therefrom, e.g., the aforementioned nucleic acid molecules (Figs. 2B, 7) and polypeptides expressed from them (Figs. 2A, 8), the invention further comprehends isolated and/or purified nucleic acid molecules and isolated and/or purified polypeptides having at least about 70%, preferably at least about 75% or about 77% identity or homology ("substantially homologous or identical"), advantageously at least about 80% or about 83%, such as at least about 85% or about 87% homology or identity ("significantly homologous or identical"), for instance at least about 90% or about 93% identity or homology ("highly homologous or identical"), more advantageously at least about 95%, e.g., at least about 97%, about 98%, about 99% or even about 100% identity or homology ("very highly homologous or identical"; or from about 84-100% identity considered "highly conserved"); and advantageously these polypeptides obtain crystal structures as herein disclosed and the nucleic acid molecules encode polypeptides that obtain crystal structures

as herein disclosed. Moreover, it is advantageous that polypeptides of the invention have greater than 98.8% identity to herein disclosed sequences, and that nucleic acid molecules of the invention have greater than 95.6% identity to herein disclosed sequences, especially as certain amino acid sequences of the invention have 98.8% identity to sequence 32 of WO01/23533 and certain nucleic acid molecules of the invention have 95.6% identity to sequence 25 of WO01/23533 (and it is intended to exclude any prior sequences). The invention also comprehends that these nucleic acid molecules and polypeptides can be used in the same fashion as the herein or aforementioned nucleic acid molecules and polypeptides.

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Nucleotide sequence homology can be determined using the "Align" program of Myers and Miller, ("Optimal Alignments in Linear Space", CABIOS 4, 11-17, 1988, incorporated herein by reference) and available at NCBI. Alternatively or additionally, the term "homology" or "identity", for instance, with respect to a nucleotide or amino acid sequence, can indicate a quantitative measure of homology between two sequences. The percent sequence homology can be calculated as $(N_{ref} - N_{dif})^*100/N_{ref}$, wherein N_{dif} is the total number of non-identical residues in the two sequences when aligned and wherein N_{ref} is the number of residues in one of the sequences. Hence, the DNA sequence AGTCAGTC will have a sequence similarity of 75% with the sequence AATCAATC $(N_{ref} = 8; N_{dif} = 2)$.

Alternatively or additionally, "homology" or "identity" with respect to sequences can refer to the number of positions with identical nucleotides or amino acids divided by the number of nucleotides or amino acids in the shorter of the two sequences wherein alignment of the two sequences can be determined in accordance with the Wilbur and Lipman algorithm (Wilbur and Lipman, 1983, PNAS, USA 80:726, incorporated herein by reference), for instance, using a window size of 20 nucleotides, a word length of 4 nucleotides, and a gap penalty of 4, and computer-assisted analysis and interpretation of the sequence data including alignment can be conveniently performed using commercially available programs (e.g., Intelligenetics TM Suite, Intelligenetics Inc. CA). When RNA sequences are said to be similar, or have a degree of sequence identity or homology with DNA sequences, thymidine (T) in the DNA sequence is considered equal to uracil (U) in the RNA sequence (see also alignment used in Figures).

RNA sequences within the scope of the invention can be derived from DNA sequences, by thymidine (T) in the DNA sequence being considered equal to uracil (U) in RNA sequences.

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Additionally or alternatively, amino acid sequence similarity or identity or homology can be determined using the BlastP program (Altschul et al., Nucl. Acids Res. 25, 3389-3402 (1997), incorporated herein by reference) and available at NCBI. The following references (each incorporated herein by reference) provide algorithms for comparing the relative identity or homology of amino acid residues of two proteins, and additionally or alternatively with respect to the foregoing, the teachings in these references can be used for determining percent homology or identity: Needleman SB and Wunsch CD, "A general method applicable to the search for similarities in the amino acid sequences of two proteins," J. Mol. Biol. 48:444-453 (1970); Smith TF and Waterman MS, "Comparison of Bio-sequences," Advances in Applied Mathematics 2:482-489 (1981); Smith TF, Waterman MS and Sadler JR, "Statistical characterization of nucleic acid sequence functional domains," Nucleic Acids Res., 11:2205-2220 (1983); Feng DF and Dolittle RF, "Progressive sequence alignment as a prerequisite to correct phylogenetic trees," J. of Molec. Evol., 25:351-360 (1987); Higgins DG and Sharp PM, "Fast and sensitive multiple sequence alignment on a microcomputer," CABIOS, 5: 151-153 (1989); Thompson JD, Higgins DG and Gibson TJ, "ClusterW: improving the sensitivity of progressive multiple sequence alignment through sequence weighing, positions-specific gap penalties and weight matrix choice, Nucleic Acid Res., 22:4673-480 (1994); and, Devereux J, Haeberlie P and Smithies O, "A comprehensive set of sequence analysis program for the VAX," Nucl. Acids Res., 12: 387-395 (1984).

In this fashion, by comprehending nucleic acid molecules and polypeptides having such homology to the particular sequences disclosed, it is envisioned that the invention encompasses homologues to the disclosed sequences, within the herein terms.

As to homologues of the disclosed amino acid sequences (Figs 2A, 8), it is advantageous that these homologues have the herein defined crystal structure; and, as to homologues of the disclosed nucleic acid sequences, it is advantageous that these homologues encode BACE proteins having the herein defined crystal structure.

Furthermore, as to inventive nucleic acid molecules, the invention comprehends codon equivalent nucleic acid molecules. For instance, if the invention comprehends "X" protein having amino acid sequence "A" and nucleic acid molecule "N" encoding protein X, the invention comprehends nucleic acid molecules that also encode protein X via one or more different codons than in nucleic acid molecule N.

In addition, as to inventive nucleic acid molecules, the invention comprehends nucleic acid molecules that hybridize under stringent conditions to herein disclosed nucleic acid molecules.

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As to herein disclosed amino acid sequences, the invention comprehends nucleic acid molecules encoding the herein disclosed amino acid sequences, as well as nucleic acid molecules that hybridize under stringent conditions to nucleic acid molecules encoding herein disclosed amino acid sequences, as these nucleic acid molecules that hybridize under stringent conditions to nucleic acid molecules encoding herein disclosed amino acid sequences can provide proteins having similarity, homology or identity as herein discussed, especially if the proteins have the same or substantially the same crystal structure as herein disclosed.

The present invention further provides in particular embodiments a crystalline structure of both the soluble BACE catalytic domain in the presence of OM99-2 and in the absence of OM99-2, both having a space group of C2 and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P21 form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand The cell dimensions of the crystals grown in the presence of OM99-2 (Figure 3A) are a= 236.63Å, b= 105.02Å, and c= 62.59Å and β =101.32° and the asymmetric unit of the crystal containing three copies of BACE. The cell dimensions of the crystals grown in the absence of OM99-2 (Figure 3B) are a= 238.3Å, b= 107.4Å, and c= 60.4Å and β =101.89°. However, as is evident from the present disclosure, the invention is not limited by the crystals having been grown in the presence or absence of OM99-2 or anything else, and that cell dimensions can vary in all directions of the cell dimensions from a stated value, e.g., a stated cell dimension value can be that value ± standard deviation (0.2Å) or ± cell variability of 3Å, and that the stated beta angle can vary, e.g., a stated beta angle can be that value, for instance 101.32° or 101.89° or that value \pm standard deviation (0.2°) or between 101° and 108°.

BACE crystals of the present invention can have a resolution better than, i.e., numerically lower than 3Å.

The present invention further provides a method of employing the crystals of the present invention in drug screening assays, comprising selecting a potential compound which binds to the active site of the BACE catalytic domain of BACE, as well as to uses of such a compound, as herein mentioned.

The present invention further provides a data storage medium encoded with the structural co-ordinates of crystallized BACE or at least a functional portion thereof. Such data storage material is capable of displaying such structures, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure co-ordinates to solve the structure of similar or homologous proteins or protein complexes. In addition, this invention relates to methods of using structure co-ordinates to screen and design compounds, including inhibitory compounds, that bind to BACE or homologues thereof. The present invention also relates to compositions and crystals of BACE in complex with a BACE inhibitor. *Cf.* WO 01/37194.

In this disclosure, "comprises," "comprising," "containing" and "having" and the like can have the meaning ascribed to them in U.S. Patent law and can mean "includes," "including," and the like; "consisting essentially of" or "consists essentially" likewise has the meaning ascribed in U.S. Patent law and the term is open-ended, allowing for the presence of more than that which is recited so long as basic or novel characteristics of that which is recited is not changed by the presence of more than that which is recited, but excludes prior art embodiments.

These and other embodiments are disclosed or are obvious from and encompassed by, the following Detailed Description.

BRIEF DESCRIPTION OF FIGURES

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The following Detailed Description, given to describe the invention by way of example, but not intended to limit the invention to specific embodiments described, may be understood in conjunction with the accompanying Figures, incorporated herein by reference, in which:

Figure 1A shows an alignment of BACE DNA sequences (EMBL-AF190725.SEQ, EMBL-AF200343.SEQ, and EMBL-AF204943.SEQ), and a BACE DNA sequence of the present invention (BACE_dna.SEQ) (SEQ ID NOs: 1-4), illustrating the novelty, nonobviousness and inventive step of the present invention*, **;

Figure 1B shows an alignment of a BACE polypeptide sequence of the present invention (baceprot.pro) and a BACE polypeptide sequence (P56817.pro) (SEQ ID NOs: 5-6), illustrating the novelty, nonobviousness and inventive step of the present invention*, **;

Figure 2A shows an inventive BACE polypeptide sequence encoded by a BACE nucleotide sequence of the present invention (SEQ ID NO: 5);

Figure 2B shows an inventive BACE nucleotide sequence (SEQ ID NO: 4);

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Figure 3A shows a photograph from a light microscope of the BACE crystal grown in the presence of OM99-2;

Figure 3B shows a photograph from a light microscope of the BACE crystal grown in the absence of any added inhibitor (OM99-2);

Figure 4A shows a diagram providing the arrangement of BACE monomers in asymmetric unit of crystallographic cell (The blue (molecule C) and orange (molecule B) molecules of the dimer, which is homologous to the dimer of Tang et al. WO01/00663, Tang et al. WO01/00665, Hong et al., Science, 2000; 290, 150-153; the molecule in pink (molecule A) forms a dimer with a crystallographically related molecule, which is homologous to the non-crystallographic dimer);

Figure 4B shows a diagram providing the packing of the molecules in the unit cell of BACE (The pink (C), orange (B) and blue molecules (A) form the asymmetric unit, which is related to the molecules in red (D), dark blue (E) and green (F) by crystallographic symmetry);

Figure 5 shows a copy of the gel from SDS-PAGE purification of BACE;

Figure 6 shows a diagrammatic representation of the comparison between the BACE protein of the present invention versus Tang et al. WO01/00663, Tang et al. WO01/00665, Hong et al., Science, 2000; 290, 150-153 (the downward facing arrows are the sites of proteolytic cleavage; TM is the transmembrane region and cyt is the cytoplasmic region), illustrating the novelty and nonobviousness and inventive step of the present invention;

Figure 7 shows an alignment of BACE DNA sequences (e.g., Ep855444.seq, WO0100663.SEQ, and WO0123533seq25.SEQ) and a BACE DNA sequence of the present invention (BACE_dna.SEQ) (SEQ ID NOs: 7-9 and 4), illustrating the novelty and nonobviousness and inventive step of the present invention*, ***;

Figure 8 shows an alignment of BACE amino acid sequences (e.g., WO0123533SEQ32.pro and WO0100663.PRO) and a BACE amino acid sequence of the present invention (baceprot.pro) (SEQ ID NOs: 10-11, and 5), illustrating the novelty and nonobviousness and inventive step of the present invention*, ***;

- (* Figure color coded to show similarities and/or differences.)
- (** EMBL-AF190725.SEQ, EMBL-AF200343.SEQ, and EMBL-AF204943.SEQ are EMBL sequences; P56817.pro is a Genbank sequence, accession P56817.)

(*** Ep855444.seq, WO0100663.SEQ, WO0123533seq25.SEQ, WO0123533SEQ32.pro and WO0100663.PRO are sequences from European Patent Application 855444, and PCT publications WO01/00663, WO01/23533, WO01/23533 and WO01/00663.)

DETAILED DESCRIPTION

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The present invention involves a catalytic domain of BACE, or a form of BACE that is suitable for crystallization with the correct disulphide bonding. Correct disulphide bonding refers to the disulphide bonding of a biologically active conformation of a catalytic domain of BACE or a BACE protein that retains functionality. Having the correct disulphide bonding eliminates the need for refolding and/or a catalytic domain of BACE or a BACE protein having an unoccupied or substantially unoccupied active site (apo-BACE crystals with no ligand bound, regardless of the source of the BACE) and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å ± standard deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or 105.02Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å ± standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°)or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P21 form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand.

The present invention further involves the expression of these BACE proteins and their use; for instance in the rational design or identification of inhibitors or modulators of BACE.

The BACE recombinant proteins of the present invention are advantageously expressed in insect cells through a baculovirus expression system and are soluble and lack glycosylation.

Increased solubility can be achieved by C-terminal truncation of the protein to remove the transmembrane and cytoplasmic regions, while glycosylation can be removed by introducing mutations at the glycosylation sites. WO01/00663 (Tang et al.), WO01/00665 (Tang et al.), Hong et al., Science, 2000; 290, 150-153, in contrast, produced the C-terminally truncated memapsin 2 protein in bacteria for crystallization. More specifically, memapsin 2 was produced as insoluble inclusion bodies in bacteria. Therefore refolding was necessary to give a soluble, active protein. However during refolding/purification the N-terminal region was lost, due to unidentified proteolytic activity. Furthermore the final protein used for crystallization studies was a mixture of species, the majority having an N-terminus at Leu41 and a minority at Leu43 (the mature Nterminus is at Glu46). See Table 4, infra, for a comparison of the Tang/Hong crystal structure with the present invention.

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The exemplified BACE protein was expressed with: 1) a His6 tag added at the C-terminus to facilitate purification; 2) mutations of the asparagine residue to glutamine in the four potential glycosylation sites at amino acids 153, 172, 223 and 354, to prevent glycosylation of the protein; 3) an N-terminus generated by furin cleavage; 4) a FLAG oligopeptide tag added to the N-terminus of the pro-peptide to enable differentiation between processed and unprocessed protein and 5) a signal peptide derived from the gp67 baculoviral protein.

Possible vectors for use in the present invention, e.g., for expressing BACE or a nucleic acid molecule encoding BACE, include, but are not limited to: for insect cells, pFastBAc1 (Life Technologies), pFastBAcDual pFastBAc1 (Life Technologies), pBlueBac III or pBlueBacHis baculovirus vectors (Invitrogen, San Diego, Calif.); for bacterial cells, pET-3 (Novagen, Madison, Wis.) and for mammalian cells, pJT4 (discussed further below), pcDNA-1 (Invitrogen, San Diego, Calif.) and pSV-SPORT 1 (Gibco-BRL, Gaithersburg, Md.). Thus, any suitable vector can be used for expression of the BACE catalytic domain or proteins or for replication and/or expression of nucleic acid molecules of the invention, including e.g., in bacterial systems such as Escherichia coli, or in viral vector systems, and DNA plasmid systems. The methods for making a vector or recombinant or plasmid for expression of BACE or nucleic acid molecules encoding BACE can be any desired method, e.g., a method which is by or analogous to the methods disclosed herein cited documents and/or in: U.S. Patent Nos. 4,603,112, 4,769,330, 5,174,993, 5,505,941, 5,338,683, 5,494,807, 4,722,848, 4,745,051, 4,879,236, 5,762,939, 5,858,368, 6,224,882, 6,103,526,

5,990,091, and 6,156,567. However, baculovirus vector systems and insect cells are presently preferred.

The expression product generated by vectors or recombinants in this invention are advantageously isolated and/or purified from infected or transfected cells or culture medium.

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The DNA sequence coding for the BACE catalytic domain can be present in the vector operably linked to regulatory elements. In one embodiment of the present invention, insect host cells are preferably transfected with the recombinant hBACE_synth_his/pFastbac baculoviral DNA, thereby resulting in expression of the BACE catalytic domain. In another embodiment of the present invention, insect host cells are preferably transfected with the FURIN/pFastBac Dual baculoviral DNA, thereby resulting in expression of furin. Transfection and co-transfection with the recombinant molecules can be effected using methods well known in the art.

Host cells may be stably transfected or transiently transfected with a recombinant expression plasmid or infected by a recombinant virus vector. The host cells include prokaryotic cells, such as *Escherichia coli*, fungal systems such as *Saccharomyces cerevisiae*, permanent cell lines derived from insects such as *Trichoplusia ni* HighFive cells, *Spodoptera frugiperda* (SF-9) cells and *Spodoptera frugiperda* (SF-21) cells, *Spodoptera frugiperda* (SF900+, U.S. Patent No. 6,103,066), and permanent mammalian cell lines such as Chinese hamster ovary (CHO) and SV40-transformed African green monkey kidney cells (COS).

The present invention contemplates "mutants" wherein a "mutant" refers to a polypeptide which is obtained by replacing at least one amino acid residue in a native or synthetic BACE catalytic domain with a different amino acid residue and/or by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native BACE catalytic domain and which has substantially the same three-dimensional structure as the native BACE catalytic domain from which it is derived. Similarly, the present invention contemplates "mimics"; e.g., proteins that have substantially the same herein disclosed crystal structure of BACE. A mimic can be a mutant. By having substantially the same three-dimensional structure is meant having a set of atomic structure co-ordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2.0Å when superimposed with the atomic structure co-ordinates of the native BACE catalytic domain from which the mutant is derived when at least about 50% to 100% of the C_{α} atoms of the native catalytic domain are included in the superposition. A mutant or mimic may have, but need not have, β -secretase activity.

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The co-ordinates of Table 5 provide a measure of atomic location in Angstroms, to a third decimal place. The co-ordinates are a relative set of positions that define a shape in three dimensions, so it is possible that an entirely different set of co-ordinates and/or space group having a different origin and/or axes and/or space group could define a similar or identical shape. Furthermore, varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the residue backbone atoms (i.e., the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues) is less than 1.5Å (preferably less than 1.0Å and more preferably less than 0.5Å) when superimposed on the co-ordinates provided in Table 5 for the residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 5 in terms of both its structural characteristics and potency for structure-based design or identification of BACE inhibitors or modulators. Likewise, changing the number and/or positions of the water molecules and/or substrate molecules of Table 5 will not generally affect the potency of the structure for structure-based design of BACE inhibitors or modulators. Thus, for the purposes described herein as being aspects of the present invention, it is within the scope of the present invention if: the Table 5 co-ordinates are transposed to a different origin and/or axes; the relative atomic positions of the atoms of the structures are varied so that the root mean square deviation of residue backbone atoms is less than 1.5Å (preferably less than 1.0Å and more preferably less than 0.5Å) when superimposed on the co-ordinates provided in Table 5 for the residue backbone atoms; and/or the number and/or positions of water molecules and/or substrate molecules is varied. Reference herein to the data of Table 5 accordingly includes the co-ordinate data in which one or more individual values of the Table are varied in this way. By "root mean square deviation" is meant the square root of the arithmetic mean of the squares of the deviations from the mean.

As used herein, "Crystal or crystalline structure" or "crystalline form": refers to a polypeptide in crystalline form. The term also includes co-crystals, as described herein. The term "co-crystal" refers to a crystal formed from a solution containing a mixture of the components i.e., polypeptide(s) and compound(s). Such compounds include, by way of example and not limitation, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc. Compounds include OM99-2, OM99-1 and a statine based peptide (Marcinkeviciene J., Luo Y., Gracian, NR., Combs Ap. And Copeland, RA. J. Biol Chem. 2001, 276:23790-23794). A soaked crystal is where a

crystal is produced from one component (polypeptide) and then the other component is soaked in the compound(s).

The "binding" which is detected between a ligand and the active site, such as to determine inhibitors of BACE is an "association" between the ligand and the active site; and "association" refers to a condition of proximity between a chemical entity or compound, or portions or fragments thereof, and the BACE catalytic domain protein, or portions or fragments thereof. The association may be non-covalent, i.e., where the juxtaposition is energetically favored by, e.g., hydrogen-bonding, van der Waals, electrostatic or hydrophobic interactions, or it may be covalent.

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The "active site" refers to that site in BACE domains where substrate peptide binding and cleavage occur. It is the site in BACE that is sought to be blocked by an inhibitor or ligand. A "functional portion" of a BACE protein includes at least the active site.

A "crystallographically-related dimer" is a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer coincide with the symmetry axes or planes of the crystal lattice, whereas a "non-crystallographically-related dimer" is a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer do not coincide with the symmetry axes or planes of the crystal lattice. And, "Bilobal structure:" refers to two globular lobes of the BACE protein and corresponds to the amino- and carboxy-terminal halves of the protein.

BACE contains a signal sequence, a pro-peptide, a catalytic aspartyl protease domain, a transmembrane region and a C-terminal cytoplasmic region. During transit through the endoplasmic reticulum, BACE undergoes constitutive N-terminal processing in the Golgi apparatus in which the pro-peptide is cleaved by a furin-like protease (Bennet et al 2000, Creemers et al 2001). More specifically, BACE undergoes a series of post-translational modifications including glycosylation, disulfide bond formation and propeptide processing. Haniu et al. have shown that BACE is N-glycosylated at four sites (Asn-153, Asn-172, Asn-223 and Asn-354) and that six Cys residues in the ectodomain form three intramolecular disulphide bonds (Cys216-Cys420, Cys278-Cys333 and Cys330-Cys380).

The present invention relates to crystalline polypeptides corresponding to the catalytic domain of BACE. Preferably, the crystalline catalytic domains are of sufficient quality to allow the determination of the three-dimensional X-ray diffraction structure to a resolution of better than, i.e., numerically lower than, 3.0Å. The invention also relates to methods for preparing and crystallizing

the polypeptides. The polypeptides themselves, as well as information derived from their crystal structures can be used to analyze and modify BACE as well as to identify compounds that interact with the catalytic domain. This can allow for the rational design or identification of compounds that inhibit or modulate BACE or interact with BACE or associate with BACE; which compounds have therapeutic value.

10 Crystalline BACE

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The crystals of the invention generally comprise substantially pure polypeptides corresponding to the BACE catalytic domain in crystalline form.

It is to be understood that the crystalline BACE catalytic domains of the invention are not limited to synthetic BACE domains. Indeed, the crystals of the invention also include native BACE catalytic domains and mutants and mimics of the BACE catalytic domain.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the BACE domain will depend, in part, on the region of the BACE domain where the substitution, addition or deletion occurs. In highly variable regions of the molecule, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are well-known in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative amino acid substitutions are well known in the art.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a BACE catalytic domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, etc. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the BACE catalytic domain will be apparent to those having skills in the art.

It should be noted that the mutants contemplated herein need not exhibit enzymatic activity. Indeed, amino acid substitutions, additions or deletions that interfere with the β-secretase activity of the BACE domain but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure co-ordinates obtained therefrom, can be used to identify compounds that bind to the native domain.

The co-crystals of the invention generally comprise a crystalline BACE domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc.

Production of Polypeptides

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The synthetic and mutated BACE catalytic domain polypeptides described herein may be chemically synthesized in whole or part using techniques that are well-known in the art (see, e.g., Kochendoerfer GG (2001) "Chemical protein synthesis methods in drug discovery". Current Opinion in Drug Discovery and Development 4, 205-214). Alternatively, methods which are well known to those skilled in the art can be used to construct expression vectors containing the synthetic or mutated BACE domain polypeptide coding sequence and appropriate transcriptional/translational control signals. These methods include in vitro recombinant DNA techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989.

A variety of host-expression vector systems may be utilized to express the synthetic BACE domain coding sequence. These include but are not limited to insect cell systems infected with recombinant virus (e.g., baculovirus) containing the BACE domain coding sequence or animal cell systems; microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the BACE domain coding sequence and yeast transformed with recombinant yeast expression vectors containing the BACE domain coding sequence. The expression elements of these systems vary in their strength and specificities. Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; in bacterial systems, inducible promoters such as pL of

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bacteriophage .mu., plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used and when generating cell lines that contain multiple copies of the BACE catalytic domain DNA, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

Crystallization Of Polypeptides And Characterization Of Crystal Structure

The crystals of the invention can be obtained by conventional means as are well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see, e.g., McPherson, 1982; McPherson, 1990; Webber, 1991).

Generally, the crystals of the invention are grown by dissolving substantially pure synthetic BACE domain polypeptide in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

In a preferred embodiment of the invention, native crystals are grown by vapor diffusion in hanging drops (McPherson, 1982 and 1990). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, equal volumes of a substantially pure polypeptide solution are mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of the reservoir. The sealed container is allowed to stand, usually for about 2-6 weeks, until crystals grow.

Thus, the invention provides a method for crystallizing BACE which comprises producing a BACE protein, e.g., by recombinant production via a suitable host and/or vector such as through expression in insect cells, recovering the BACE and growing crystals from the recovered BACE. The BACE so produced is suitable for X-ray diffraction analysis. And, the growing of the crystals can be by any suitable means, advantageously the hanging drop method.

Uses of the Crystals and Atomic Structure Co-ordinates

The crystals of the invention, and particularly the atomic structure co-ordinates obtained therefrom, have a wide variety of uses. The crystals (either apo or co-complexed) and structure co-

ordinates (either apo or co-complexed) are particularly useful for identifying compounds that inhibit β -secretase activity as an approach towards developing new therapeutic agents.

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The structure co-ordinates described herein can be used as phasing models in determining the crystal structures of additional synthetic or mutated BACE domains, as well as the structures of co-crystals of such domains with ligands such as inhibitors, agonists, antagonists, etc. The structure co-ordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of synthetic or mutated BACE domains, such as those obtained via nuclear magnetic resonance (NMR).

The provision of the structure of BACE crystals in Table 5 provides the skilled artisan with a detailed insight into the mechanisms of action of BACE. This insight provides a means to design inhibitors of BACE which can be used for inhibiting BACE or the production of A β or fragments thereof or treating AD or disorders involving the production of A β or fragments thereof (which disorders are treatable by inhibition of BACE) in an individual in need thereof.

The provision of the crystal structure of BACE allows a novel approach for drug discovery, identification, and design for modulators, e.g., inhibitors, of BACE. Accordingly, the invention provides a computer-based method of rational drug design or identification which comprises: providing the structure of BACE as defined by the co-ordinates or the identifying co-ordinates in Table 5; providing a structure of a candidate modulator or inhibitor; and fitting the structure of the candidate to the structure of BACE of Table 5.

In an alternative aspect, the method may use the co-ordinates of atoms of interest of BACE which are in the vicinity of the active site or binding region in order to model the pocket in which the substrate or ligand binds. These co-ordinates may be used to define a space which is then screened "in silico" against a candidate modulator molecule. Thus, the invention provides a computer-based method of rational drug design or identification which comprises: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"); providing the structure of a candidate modulator or inhibitor; and fitting the structure of the candidate to the selected co-ordinates of BACE.

In practice, it may be desirable to model a sufficient number of atoms of BACE as defined by the co-ordinates of Table 5 which represent the active site or binding region. Thus, there can be provided the co-ordinates of at least 5, advantageously at least 10, more advantageously at least 50 and even more advantageously at least 100 atoms of the BACE structure.

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Accordingly, the methods of the invention can employ a sub-domain of interest of BACE which is in the vicinity of the active site or binding region, and the invention can provide a computer-based method for identifying or rationally designing a drug which comprises: providing the co-ordinates of at least a sub-domain of BACE; providing the structure of a candidate modulator or inhibitor of BACE; and fitting the structure of the candidate to the co-ordinates of the BACE sub-domain provided.

These methods can optionally include synthesizing the candidate and can optionally further include contacting the candidate with BACE to test whether there is binding and/or inhibition.

"Fitting" can mean determining, by automatic or semi-automatic means, interactions between at least one atom of the candidate and at least one atom of BACE and calculating the extent to which such an interaction is stable. Interactions can include attraction, repulsion, brought about by charge, steric considerations, and the like. A "sub-domain" can mean at least one, e.g., one, two, three, or four, complete element(s) of secondary structure. Particular regions of BACE include those identified in Table 5.

Modulators of BACE may be inhibitors of BACE or compounds which affect its specificity or activity in other ways. Advantageously, modulators are inhibitors.

The step of providing the structure of a candidate modulator molecule may involve selecting the compound by computationally screening a database of compounds for interaction with the active site. For example, a 3-D descriptor for the potential modulator may be derived, the descriptor including geometric and functional constraints derived from the architecture and chemical nature of the active site. The descriptor may then be used to interrogate the compound database, a potential modulator being a compound that has a good match to the features of the descriptor. In effect, the descriptor can be a type of virtual pharmacophore.

In any event, the determination of the three-dimensional structure of BACE provides a basis for the design of new and specific modulators for BACE. For example, from knowing the three-dimensional structure of BACE, computer modelling programs may be used to design or identify different molecules expected to interact with possible or confirmed active sites such as binding sites or other structural or functional features of BACE.

More specifically, a potential modulator of BACE activity can be examined through the use of computer modeling using a docking program such as GRAM, DOCK or AUTODOCK (see Walters et al. Drug Discovery Today, vol. 3, no. 4 (1998), 160-178, and Dunbrack et al. Folding

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and Design 2 (1997), 27-42) to identify potential inhibitors of BACE. This procedure can include computer fitting of potential modulators to BACE to ascertain how well the shape and the chemical structure of the potential modulator (e.g., inhibitor) will bind to the enzyme.

Also, computer-assisted, manual examination of the active site or binding site of BACE may be performed. The use of programs such as GRID (P. Goodford, J. Med. Chem, 1985, 28, 849-57) – program that determines probable interaction sites between molecules with various functional groups and the enzyme surface – may also be used to analyze the active site or binding site to predict partial structures of modulating compounds.

Computer programs can be employed to estimate the attraction, repulsion or steric hindrance of the two binding partners, e.g., BACE and a candidate inhibitor. Generally, the tighter the fit, the fewer the steric hindrances, and the greater the attractive forces, the more potent the potential modulator, since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a candidate modulator, the more likely it is that it will not interact with other proteins as well. This will tend to minimize potential side-effects due to unwanted interactions with other proteins.

In a further aspect the invention provides for a method for determining the structure of a modulator of BACE bound to BACE, said method comprising, (a) providing a crystal of BACE according to the invention, (b) soaking the crystal with said modulator; and (c) determining the structure of said BACE-modulator complex.

The invention further involves, in place of or in addition to *in silico* methods, high throughput screening of compounds to select compounds with binding activity. Those compounds which show binding activity may be selected as possible candidate modulators, and further crystallized with BACE, e.g., by co-crystallization or by soaking, for X-ray analysis. The resulting X-ray structure may be compared with that of Table 5 for a variety of purposes. For example, where the contacts made by such compounds overlap with those made by BACE, novel molecules comprising residues which contain contacts of BACE and other compounds may be provided.

Having designed, identified, or selected possible binding candidate modulators or inhibitors by determining those which have favorable fitting properties, e.g., strong attraction between a candidate and BACE, these can be then screened for activity. Consequently, the invention further involves: obtaining or synthesizing the candidate modulator or inhibitor; and contacting the candidate modulator or inhibitor with BACE to determine the ability of the candidate to inhibit or

modulate or interact with BACE. In the latter step, the candidate is advantageously contacted with BACE under conditions to determine its function. Instead of, or in addition to, performing such an assay, the invention may comprise: obtaining or synthesizing the candidate modulator, forming a complex of BACE and the candidate, and analyzing the complex, e.g., by X-ray diffraction or NMR or other means, to determine the ability of the candidate to interact with BACE. Detailed structural information can then be obtained about the binding of the candidate to BACE, and in light of this information, adjustments can be made to the structure or functionality of the potential modulator, e.g., to improve its binding to BACE. These steps may be repeated and re-repeated as necessary. Advantageously, in the contacting step, the potential modulator is contacted with BACE in the presence of a substrate and typically a buffer, to determine the ability of the potential modulator to alter the function of BACE.

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The invention further involves a method of determining three dimensional structures of BACE homologues of unknown structure by using the structural co-ordinates of Table 5. For example, if X-ray crystallographic or NMR spectroscopic data is provided for a BACE homologue of unknown structure, the structure of BACE as defined in Table 5 may be used to interpret that data to provide a likely structure for the BACE homologue by techniques well known in the art, e.g., by phase modeling in the case of X-ray crystallography. Thus, an inventive method can comprise: aligning a representation of an amino acid sequence of a BACE homologue of unknown structure with the amino acid sequence of BACE to match homologous regions of the amino acid sequences; modeling the structure of the matched homologous regions of the BACE of unknown structure on the structure as defined in Table 5 of the corresponding regions of BACE; and, determining a conformation (e.g. so that favorable interactions are formed within the BACE of unknown structure and/or so that a low energy conformation is formed) for the BACE of unknown structure which substantially preserves the structure of said matched homologous regions. "Homologous regions" describes amino acid residues in two sequences that are identical or have similar, e.g., aliphatic, aromatic, polar, negatively charged, or positively charged, side-chain chemical groups. Identical and similar residues in homologous regions are sometimes described as being respectively "invariant" and "conserved" by those skilled in the art. Advantageously, the first and third steps are performed by computer modeling. Homology modeling is a technique that is well known to those skilled in the art (see, e.g., Greer, Science vol. 228 (1985) 1055, and Blundell et al. Eur J Biochem vol 172 (1988), 513).

In general, comparison of amino acid sequences is accomplished by aligning an amino acid sequence of a polypeptide of a known structure with the amino acid sequence of a the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous are grouped together. This method detects conserved regions of the polypeptides and accounts for amino acid insertions and deletions. Homology between amino acid sequences can be determined by using commercially available algorithms. In addition to those otherwise mentioned herein, mention is made too of the programs BLAST, gapped BLAST, BLASTN, and PSI-BLAST, provided by the National Center for Biotechnology Information. These programs are widely used in the art for this purpose and can align homologous regions of two amino acid sequences.

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Once the amino acid sequence of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in a computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure. The structures of amino acids located in non-conserved regions may be assigned manually using standard peptide geometries or by molecular simulation techniques, such as molecular dynamics. Refining the entire structure can be by molecular dynamics and/or energy minimization.

The aspects of the invention which employ the BACE structure *in silico* may be equally applied to homologue models of BACE obtained by the above aspect of the invention and this forms yet a further embodiment of the invention. Thus, having determined a conformation of a BACE by the methods described herein, such a conformation may be used in a computer-based method of rational drug or compound design or identification as described herein.

The invention further provides a method for determining the structure of a modulator of BACE bound to BACE comprising: providing a crystal of BACE, e.g., according to the invention, soaking the crystal with the modulator, and determining the structure of the BACE-modulator complex. Alternatively or additionally the BACE and the modulator may be co-crystallized.

Having obtained and characterized a modulator according to the invention, the invention further provides a method for modulating the activity of BACE which comprises: providing BACE under conditions where, in the absence of a modulator, BACE is able to exhibit secretase activity,

providing a modulator compound (e.g., contacting the modulator and the BACE), determining the extent to which the activity of BACE is altered by the presence of the modulator compound.

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The invention further provides systems, such as computer systems, intended to generate structures and/or perform rational drug design for a BACE or complex of BACE and a potential modulator. The system can contain: atomic co-ordinate data according to Table 5 or derived therefrom by homology modeling, said data defining the three-dimensional structure of a BACE or at least one sub-domain thereof; or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5. The invention also involves computer readable media with: atomic co-ordinate data according to Table 5 or derived therefrom by homology modeling, said data defining the three-dimensional structure of a BACE or at least one sub-domain thereof; or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5. "Computer readable media" refers to any media which can be read and accessed directly by a computer, and includes, but is not limited to: magnetic storage media such as floppy discs, hard storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM and ROM; and hybrids of these categories, such as magnetic/optical media. By providing such computer readable media, the atomic co-ordinate data can be routinely accessed to model BACE or a subdomain thereof. For example RASMOL (Sayle et al., TIBS vol. 20 (1995), 374) is a publicly available software package which allows access and analysis of atomic co-ordinate data for structural determination and/or rational drug design. The invention further comprehends methods of doing business by providing access to such computer readable media and/or computer systems and/or atomic co-ordinate data to users; e.g., the media and/or atomic co-ordinate data can be accessible to a user, for instance on a subscription basis, via the Internet or a global communication/computer network; or, the computer system can be available to a user, on a subscription basis. Structure factor data, which are derivable from atomic co-ordinate data (see, e.g., Blundell et al., in Protein Crystallography, Academic Press, NY, London and San Francisco (1976)), are particularly useful for calculating, e.g., difference Fourier electron density maps. Thus, there are additional uses for the computer readable media and/or computer systems and/or atomic co-ordinate data and additional reasons to provide them to users. A "computer system" refers to the hardware means, software means and data storage means used to analyze the atomic co-ordinate data of the present invention. The minimum hardware means of computer-based

systems of the invention may comprise a central processing unit (CPU), input means, output means, and data storage means. Desirably, a monitor is provided to visualize structure data. The data storage means may be RAM or other means for accessing computer readable media of the invention. Examples of such systems are microcomputer workstations available from Silicon Graphics Incorporated and Sun Microsystems running Unix based, Windows NT or IBM OS/2 operating systems.

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The invention also provides a method of analyzing a complex of BACE and a potential modulator comprising: employing X-ray crystallographic diffraction data from the complex and a three-dimensional structure of BACE or at least a sub-domain thereof, to generate a difference Fourier electron density map of the complex; advantageously, the three-dimensional structure being as defined by the atomic co-ordinate data according to Table 5.

Such complexes can be crystallized and analyzed using X-ray diffraction methods, e.g., according to the approaches described by Greer et al., J of Medicinal Chemistry, vol 37 (1994), 1035-54, and difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallized BACE and the solved structure of uncomplexed BACE. These maps can then be used to determine whether and where a particular potential modulator binds to BACE and/or changes the conformation of BACE. Electron density maps can be calculated using programs such as those from the CCP4 computer package (Collaborative Computing Project, No. 4. The CCP4 Suite: Programs for Protein Crystallography, Acta Crystallographica, D50, 1994, 760-763). For map visualization and model building programs such as "QUANTA" (1994, San Diego, CA: Molecular Simulations, Jones et al., Acta Crystallography A47 (1991), 110-119) can be used.

Table 5 gives atomic co-ordinate data for BACE complexed with OM99-2, and lists each atom by a unique number; the chemical element and its position in each amino acid residue, the amino acid residue in which the element is located, the chain identifier, the number of the residue, co-ordinates (e.g., X, Y, Z) which define with respect to the crystallographic axes the atomic position (in Å) of the respective atom, the occupancy of the atom in the respective position, "B", isotropic displacement parameter (in Å²) which accounts for movement of the atom around its atomic center, and atomic number.

Determination of the 3D structure of BACE provides important information about the likely active site(s) of BACE, particularly when comparisons are made with other enzymes, such as

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similar enzymes. This information may be used for rational design of BACE inhibitors, e.g., by computational techniques that identify possible binding ligands for the active site(s), by enabling linked-fragment approaches to drug design, and by enabling the identification and location of bound ligands using analyses such as X-ray crystallographic analysis.

Greer et al., *supra*, relates to an iterative approach to ligand design based on repeated sequences of computer modeling, protein-ligand complex formation, and X-ray analysis. Thymidylate synthase inhibitors were designed by Greer; and, BACE inhibitors may also be designed in this way. Using, for example, GRID (P. Goodford, J. Med. Chem, 1985, 28, 849-57) or the solved 3D structure of BACE, a potential modulator of BACE may be designed that complements the functionalities of the BACE active site(s). The potential modulator can be synthesized, formed into a complex with BACE, and the complex then analyzed, e.g., by X-ray crystallography, NMR or a combination thereof, to identify the actual position of the bound compound.

Determination of the position of the potential modulator compound in the complex allows determination of the interactions of it with BACE. This allows the skilled artisan to analyze the affinity and specificity of the compound for BACE, and to propose modifications to the compound to increase or decrease either or both of these properties. Thus, the structure and/or functional groups of the compound can then be adjusted, if necessary or desired, in view of the results from the analysis (e.g., X-ray analysis), and the synthesis and analysis sequence repeated until an optimized compound is obtained. Related approaches to structure-based drug design are also discussed in other documents cited herein, as well as in Bohacek et al., Medicinal Research Reviews, vol. 16 (1996), 3-5.

As a result of the determination of the BACE 3D structure, more purely computational techniques for rational drug design may also be used to design BACE modulators; for example, automated ligand-receptor docking programs (see Jones et al., in Current Opinion in Biotechnology, vol 6 (1995), 652-656) which require accurate information on the atomic coordinates of target receptors, may be used to design or identify potential BACE modulators or inhibitors.

Linked-fragment approaches to drug design also require accurate information on the atomic co-ordinates of a target. Small compounds that have the potential to bind to regions of BACE which in themselves may not be modulator compounds may be assembled by chemical linkage to

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provide potential modulators. Thus, the basic idea behind these approaches is to determine the binding locations of more than one, e.g., plural or a plurality of, ligands to a target molecule, and then construct a molecular scaffold to connect the ligands together in such a way that their relative binding positions are preserved. The ligands may be provided computationally and modeled in a computer system, or provided in an experimental setting, wherein crystals according to the invention are provided and more than one, e.g., plural or a plurality of, ligands soaked separately or -10 in mixed pools into the crystal prior to analysis, e.g., X-ray analysis, and determination of their location.

The binding site of two or more ligands are determined and may be connected to thus form a potential lead compund that can be further refined, e.g., the iterative technique of Greer et al. For a virtual linked-fragment approach, see Verlinde et al., J of Computer-Aided Molecular Design 6 (1992), 131-147 and for NMR and X-ray approaches, see Skuker et al., Science 274 (1996), 1531-1534, and Stout et al., Structure 6 (1998), 839-48. The use of these or other approaches to design and/or identify BACE modulators (see, e.g., patent documents cited herein such as in the Background Section, supra) is made possible by the determination of the BACE structure.

Many of the techniques and approaches to structure-based described herein employ X-ray analysis to identify the binding position of a potential modulator in a complex with a protein. A common way of doing this is to perform X-ray crystallography on the complex, produce a difference Fourier electron density map, and associate a particular pattern of electron density with the potential modulator. However, to produce a map (See Blundell et al., supra), it is important to know the 3D structure of the protein beforehand (or at least the protein structure factors). Therefore, determination of the BACE structure also allows difference Fourier electron density maps of complexes of BACE with a potential modulator to be produced, which can greatly assist in the process of rational compound and/or drug design or identification.

The approaches to structure-based drug or compound design or identification described herein involve initial identification of possible compounds for interaction with the target molecule (in this case BACE). Sometimes these compounds are known, e.g., from research literature. However, when they are not, or when novel compounds are wanted, a first stage of the drug or compound design or identification program may involve computer-based in silico screening of compound databases (such as the Cambridge Structural Database) with the aim of identifying compounds which interact with the active site or sites of the target bio-molecule (in this case

BACE). Screening selection criteria may be based on pharmacokinetic properties such as metabolic stability and toxicity. However, determination of the BACE structure allows the architecture and chemical nature of each BACE active site to be identified, which in turn allows the geometric and functional constraints of a descriptor for the potential inhibitor to be derived. The descriptor can be, therefore, a type of virtual 3D pharmacophore, which can also be used as selection criteria or filter for database screening.

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Compounds which have a chemical structure selected using the invention, wherein said compounds are BACE modulators or inhibitors, form a further aspect of the invention; and, such compounds may be used in methods of medical treatments, such as for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD or other maladies involving BACE or the production of $A\beta$ or fragments thereof. Further, such compounds may be used in the preparation of medicaments for such treatments. The compounds may be employed alone or in combination with other treatments for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD or other maladies involving BACE or the production of $A\beta$ or fragments thereof; and, the compounds may be used in the preparation of combination medicaments for such treatments, or in kits containing the compound and the other treatment.

Turning more specifically to BACE, BACE is a pepsin-like aspartyl proteinase, the mature enzyme consisting of the N-terminal catalytic domain, a transmembrane domain, and a small cytoplasmic domain. BACE has an optimum activity at pH 4.5 (Vassar et al., 1999) or pH 5.0 (Yan et al. 1999) and is found in acidic subcellular compartments such as golgi and endosomes (Vassar et al., 1999 and Capell et al., 2000). The pH in the endosome and trans golgi network, where BACE appears to function, fluctuates in the range of pH 4.5 - 6.0 with the average pH being stated as 5.0 (Lee et al. 1996) and pH 5.4 (Overly et al. 1995). BACE is not inhibited by standard pepsin inhibitors such as pepstatin. It has been shown that the catalytic domain minus the transmembrane and cytoplasmic domain has activity against substrate peptides (Lin et al, 2000). Consequently, this soluble catalytic domain is suitable for crystallization studies and a crystal structure of this will give a representative structure of the BACE active site for the design of inhibitor molecules. Ideally it would be desirable to crystallize a form of BACE with an unoccupied active site. This could be used to soak in small molecule inhibitors of the enzyme and to investigate their binding modes. Crystals of BACE grown both in the presence and absence of inhibitor, having same space group and similar unit cell parameters are described. These crystals are grown between pH 5.6 and

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pH 5.8 and thus are grown at the biologically relevant pH of BACE. This is also close to the optimum pH of the enzyme. Upon soaking the C2 crystal form with a ligand, some reorganization of the molecules in the crystal will take place, resulting in a space group change from C2 to P2₁. The cell dimensions and the packing of the P2₁ form are closely related to those of the C2 form. Because the BACE crystals are grown at physiologically relevant pH the compounds identified in accordance with the invention would be of more biological relevance. The lead compounds/inhibitors generated may be of higher therapeutic value and would truly reflect the mode of inhibition *in vivo*, particularly for those compounds that are susceptible to changes in protonation state.

A synthetic gene encoding the pro- and aspartyl protease domains of BACE was constructed (see Example 1). The construct extended from Thr 22 to Ser 453 (numbering refers to the full-length BACE sequence, e.g. Genbank accession P56817, SEQ ID NO:6). In each of the four potential glycosylation sites (Asn-X-Ser/Thr: Asparagines-153, -172, -223 and -354) the Asparagine residue was mutated to Glutamine to prevent glycosylation of the protein. Silent mutations were also introduced into the coding sequence in order to reduce the GC content of the gene (Figure 1A shows an alignment of the synthetic DNA sequence of the present invention with other wild-type BACE genes). A His6 peptide tag was added to the C-terminus of the protein sequence to facilitate purification on Nickel agarose (see Example 1).

Both forms of the protein could be detected using an anti-His6 antibody (see Figure 5); only the unprocessed form containing the pro-peptide was detected using an anti-FLAG antibody. Further changes to the synthetic BACE catalytic domain sequence were the addition of the baculoviral gp67 signal sequence instead of the BACE signal, the addition of a FLAG tag to the N-terminus of the pro-peptide. The gp67 signal sequence increased the secretion of the protein into the cell culture medium, and the FLAG tag was added to allow differentiation between species arising from incomplete pro-peptide cleavage (and to determine if separation is required) (see Figure 6). Insect cells infected with the BACE baculovirus secreted a mixture of processed and unprocessed BACE into the culture medium. Figure 2A shows the polypeptide sequence encoded by the synthetic BACE gene.

As mentioned previously, the invention comprehends the use of the inventive BACE proteins in assays or methods for determining inhibitors thereof, e.g., compounds, compositions or active agents or ingredients that bind to BACE, advantageously irreversibly, preferably so as to

have a therapeutic effect with respect to AD and other maladies. After determination of a suitable compound, composition, active agent or ingredient that binds to BACE, the compound, composition, active agent or ingredient is then formulated into a composition for administration and is administered to a subject in need thereof. These therapeutics can be administered in known formulations, by known routes of administration, following the teachings of documents cited herein.

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It is noted that these therapeutics can be a chemical compound and/or antibody and/or portion thereof or a pharmaceutically acceptable salt and can be administered alone or as an active ingredient in combination with pharmaceutically acceptable carriers, diluents, and vehicles, as well as other active ingredients.

The compounds can be administered orally, subcutaneously or parenterally including intravenous, intraarterial, intramuscular, intraperitoneally, and intranasal administration as well as intrathecal and infusion techniques.

It is noted that humans are treated generally longer than the mice or other experimental animals which treatment has a length proportional to the length of the disease process and drug effectiveness. The doses may be single doses or multiple doses over a period of several days, but single doses are preferred. Thus, one can scale up from animal experiments, e.g., rats, mice, and the like, to humans, by techniques from this disclosure and documents cited herein and the knowledge in the art, without undue experimentation.

The treatment generally has a length proportional to the length of the disease process and drug effectiveness and the patient being treated.

When administering a therapeutic of the present invention parenterally, it will generally be formulated in a unit dosage injectable form (solution, suspension, emulsion). The pharmaceutical formulations suitable for injection include sterile aqueous solutions or dispersions and sterile powders for reconstitution into sterile injectable solutions or dispersions. The carrier can be a solvent or dispersing medium containing, for example, water, ethanol, polyol (for example, glycerol, propylene glycol, liquid polyethylene glycol, and the like), suitable mixtures thereof, and vegetable oils.

Proper fluidity can be maintained, for example, by the use of a coating such as lecithin, by the maintenance of the required particle size in the case of dispersion and by the use of surfactants. Nonaqueous vehicles such a cottonseed oil, sesame oil, olive oil, soybean oil, corn oil, sunflower

oil, or peanut oil and esters, such as isopropyl myristate, may also be used as solvent systems for compound compositions

Additionally, various additives which enhance the stability, sterility, and isotonicity of the compositions, including antimicrobial preservatives, antioxidants, chelating agents, and buffers, can be added. Prevention of the action of microorganisms can be ensured by various antibacterial and antifungal agents, for example, parabens, chlorobutanol, phenol, sorbic acid, and the like. In many cases, it will be desirable to include isotonic agents, for example, sugars, sodium chloride, and the like. Prolonged absorption of the injectable pharmaceutical form can be brought about by the use of agents delaying absorption, for example, aluminum monostearate and gelatin. According to the present invention, however, any vehicle, diluent, or additive used would have to be compatible with the compounds.

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Sterile injectable solutions can be prepared by incorporating the compounds utilized in practicing the present invention in the required amount of the appropriate solvent with various amounts of the other ingredients, as desired.

A pharmacological formulation of the present invention, e.g., comprising a therapeutic compound, can be administered to the patient in an injectable formulation containing any compatible carrier, such as various vehicles, adjuvants, additives, and diluents; or the compounds utilized in the present invention can be administered parenterally to the patient in the form of slow-release subcutaneous implants or targeted delivery systems such as monoclonal antibodies, iontophoretic, polymer matrices, liposomes, and microspheres.

A pharmacological formulation of the compound utilized in the present invention can be administered orally to the patient. Conventional methods such as administering the compounds in tablets, suspensions, solutions, emulsions, capsules, powders, syrups and the like are usable. Known techniques which deliver the compound orally or intravenously and retain the biological activity are preferred.

In one embodiment, a formulation of the present invention can be administered initially, and thereafter maintained by further administration. For instance, a formulation of the invention can be administered in one type of composition and thereafter further administered in a different or the same type of composition. For example, a formulation of the invention can be administered by intravenous injection to bring blood levels to a suitable level. The patient's levels are then

maintained by an oral dosage form, although other forms of administration, dependent upon the patient's condition, can be used.

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The quantity to be administered will vary for the patient being treated and will vary from about 100 ng/kg of body weight to 100 mg/kg of body weight per day and preferably will be from 10 pg/kg to 10 mg/kg per day. For instance, dosages can be readily ascertained by those skilled in the art from this disclosure and the knowledge in the art. Thus, the skilled artisan can readily determine the amount of compound and optional additives, vehicles, and/or carrier in compositions and to be administered in methods of the invention. Typically, an adjuvant or additive is commonly used as 0.001 to 50 wt% solution in phosphate buffered saline, and the active ingredient is present in the order of micrograms to milligrams, such as about 0.0001 to about 5 wt%, preferably about 0.0001 to about 1 wt%, most preferably about 0.0001 to about 0.05 wt% or about 0.001 to about 20 wt%, preferably about 0.01 to about 10 wt%, and most preferably about 0.05 to about 5 wt%. Of course, for any composition to be administered to an animal or human, and for any particular method of administration, it is preferred to determine therefor: toxicity, such as by determining the lethal dose (LD) and LD₅₀ in a suitable animal model e.g., rodent such as mouse; and, the dosage of the composition(s), concentration of components therein and timing of administering the composition(s), which elicit a suitable response, such as by titrations of sera and analysis thereof. Such determinations do not require undue experimentation from the knowledge of the skilled artisan, this disclosure and the documents cited herein. And, the time for sequential administrations can be ascertained without undue experimentation.

Examples of compositions comprising a therapeutic of the invention include liquid preparations for orifice, e.g., oral, nasal, anal, vaginal, peroral, intragastric, mucosal (e.g., perlingual, alveolar, gingival, olfactory or respiratory mucosa) etc., administration such as suspensions, syrups or elixirs; and, preparations for parenteral, subcutaneous, intradermal, intramuscular or intravenous administration (e.g., injectable administration), such as sterile suspensions or emulsions. Such compositions may be in admixture with a suitable carrier, diluent, or excipient such as sterile water, physiological saline, glucose or the like. The compositions can also be lyophilized. The compositions can contain auxiliary substances such as wetting or emulsifying agents, pH buffering agents, gelling or viscosity enhancing additives, preservatives, flavoring agents, colors, and the like, depending upon the route of administration and the preparation desired. Standard texts, such as "REMINGTON'S PHARMACEUTICAL SCIENCE",

17th edition, 1985, incorporated herein by reference, may be consulted to prepare suitable preparations, without undue experimentation.

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Compositions of the invention, are conveniently provided as liquid preparations, e.g., isotonic aqueous solutions, suspensions, emulsions or viscous compositions which may be buffered to a selected pH. If digestive tract absorption is preferred, compositions of the invention can be in the "solid" form of pills, tablets, capsules, caplets and the like, including "solid" preparations which are time-released or which have a liquid filling, e.g., gelatin covered liquid, whereby the gelatin is dissolved in the stomach for delivery to the gut. If nasal or respiratory (mucosal) administration is desired, compositions may be in a form and dispensed by a squeeze spray dispenser, pump dispenser or aerosol dispenser. Aerosols are usually under pressure by means of a hydrocarbon. Pump dispensers can preferably dispense a metered dose or, a dose having a particular particle size.

Compositions of the invention can contain pharmaceutically acceptable flavors and/or colors for rendering them more appealing, especially if they are administered orally. The viscous compositions may be in the form of gels, lotions, ointments, creams and the like (e.g., for transdermal administration) and will typically contain a sufficient amount of a thickening agent so that the viscosity is from about 2500 to 6500 cps, although more viscous compositions, even up to 10,000 cps may be employed. Viscous compositions have a viscosity preferably of 2500 to 5000 cps, since above that range they become more difficult to administer. However, above that range, the compositions can approach solid or gelatin forms which are then easily administered as a swallowed pill for oral ingestion.

Liquid preparations are normally easier to prepare than gels, other viscous compositions, and solid compositions. Additionally, liquid compositions are somewhat more convenient to administer, especially by injection or orally. Viscous compositions, on the other hand, can be formulated within the appropriate viscosity range to provide longer contact periods with mucosa, such as the lining of the stomach or nasal mucosa.

Obviously, the choice of suitable carriers and other additives will depend on the exact route of administration and the nature of the particular dosage form, e.g., liquid dosage form (e.g., whether the composition is to be formulated into a solution, a suspension, gel or another liquid form), or solid dosage form (e.g., whether the composition is to be formulated into a pill, tablet, capsule, caplet, time release form or liquid-filled form).

Solutions, suspensions and gels, normally contain a major amount of water (preferably purified water) in addition to the active compound. Minor amounts of other ingredients such as pH adjusters (e.g., a base such as NaOH), emulsifiers or dispersing agents, buffering agents, preservatives, wetting agents, jelling agents, (e.g., methylcellulose), colors and/or flavors may also be present. The compositions can be isotonic, i.e., it can have the same osmotic pressure as blood and lacrimal fluid.

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The desired isotonicity of the compositions of this invention may be accomplished using sodium chloride, or other pharmaceutically acceptable agents such as dextrose, boric acid, sodium tartrate, propylene glycol or other inorganic or organic solutes. Sodium chloride is preferred particularly for buffers containing sodium ions.

Viscosity of the compositions may be maintained at the selected level using a pharmaceutically acceptable thickening agent. Methylcellulose is preferred because it is readily and economically available and is easy to work with. Other suitable thickening agents include, for example, xanthan gum, carboxymethyl cellulose, hydroxypropyl cellulose, carbomer, and the like. The preferred concentration of the thickener will depend upon the agent selected. The important point is to use an amount which will achieve the selected viscosity. Viscous compositions are normally prepared from solutions by the addition of such thickening agents.

A pharmaceutically acceptable preservative can be employed to increase the shelf-life of the compositions. Benzyl alcohol may be suitable, although a variety of preservatives including, for example, parabens, thimerosal, chlorobutanol, or benzalkonium chloride may also be employed. A suitable concentration of the preservative will be from 0.02% to 2% based on the total weight although there may be appreciable variation depending upon the agent selected.

Those skilled in the art will recognize that the components of the compositions should be selected to be chemically inert with respect to the active compound. This will present no problem to those skilled in chemical and pharmaceutical principles, or problems can be readily avoided by reference to standard texts or by simple experiments (not involving undue experimentation), from this disclosure and the documents cited herein.

The inventive compositions of this invention are prepared by mixing the ingredients following generally accepted procedures. For example the selected components may be simply mixed in a blender, or other standard device to produce a concentrated mixture which may then be adjusted to the final concentration and viscosity by the addition of water or thickening agent and

possibly a buffer to control pH or an additional solute to control tonicity. Generally the pH may be from about 3 to 7.5. Compositions can be administered in dosages and by techniques well known to those skilled in the medical and veterinary arts taking into consideration such factors as the age, sex, weight, and condition of the particular patient, and the composition form used for administration (e.g., solid vs. liquid). Dosages for humans or other mammals can be determined without undue experimentation by the skilled artisan, from this disclosure, the documents cited herein, and the knowledge in the art.

Suitable regimes for initial administration and further doses or for sequential administrations also are variable, may include an initial administration followed by subsequent administrations; but nonetheless, may be ascertained by the skilled artisan, from this disclosure, the documents cited herein, and the knowledge in the art.

Accordingly, the invention comprehends, in further aspects, methods for preparing therapeutic compositions including an active agent, ingredient or compound or BACE inhibitor as from inventive methods herein for ascertaining compounds that bind to and/or inhibit BACE, as well as to methods for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD or other maladies.

Furthermore, as discussed herein, the inventive BACE proteins are useful in generating antibodies, which are themselves useful in assays as well as in therapeutics. From documents cited herein, one can readily make and use anti-BACE antibodies and methods for producing monoclonal antibodies are well known to those of ordinary skill in the art, see, e.g., U.S. Patent No. 4,196,265 and 6,221,645. Thus, the BACE proteins of the invention can be used to generate antibodies and the antibodies can be used, without undue experimentation.

The invention will now be further described by the following non-limiting Examples, given by way of illustration.

EXAMPLES

EXAMPLE 1: Production of BACE in Insect Cells

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A. Gene Construction and Cloning

The synthetic BACE catalytic domain sequence was constructed a combination of oligonucleotide synthesis and overlap PCR (Cambridge Bioscience Ltd, Cambridge UK).

Mutations were inserted at specific sites within the BACE catalytic domain sequence during synthesis to reduce the GC content of the gene. The synthetic gene was then cut with restriction

enzymes Sal1 and Not1 to generate a 1489 bp fragment which was then subcloned into the expression vector pFastBac1 (LifeTechnologies), and the DNA sequence verified by standard DNA sequencing methods (e.g., electrophoresis and automated DNA sequence analysis of the insert).

The cDNA encoding human furin was cut by restriction enzymes to generate a 3216 bp Smal Xmal fragment that was then subcloned into the expression vector pFastBac Dual (LifeTechnologies).

B. Baculovirus Generation and Fermentation

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Recombinant baculoviruses were constructed by using the expression vectors of the Bacto-Bac™ system (LifeTechnologies), according to the manufacturers instructions. Manipulations involving insect cells and baculoviruses were carried out according to standard protocols (King and Possee, 1992).

As it has been shown that coexpression of the prohormone convertase furin increases expression of mature TGF-β in insect cells (Laprise et al., 1998), the effect of furin co-expression on BACE production was evaluated i.e., while the total amount of BACE produced did not increase with furin coespression, there was a reproducible increase in the fraction of processed protein from about 30% of total BACE up to about 60%; this result is quite surprising and advantageous.

Trichoplusia ni HighFive cells (Invitrogen, Carlsbad CA,USA) were found to give higher levels of BACE expression than Spodoptera frugiperda Sf9 cells, and were used for all protein production. Protein production was carried out in a 20-30 liter working volume bioreactor (Applikon Dependable Instruments, Schiedam, Netherlands), containing Excell 405 medium (JRH Scientific). Cells were infected at a multiplicity of infection (MOI) of 0.1 of each virus at a cell density of 1.5x10⁶ cells/ml. Glucose concentration was measured during the fermentation and adjusted to maintain the starting concentration. Three days after viral infection the HighFive cells were cleared from the medium by continuous flow centrifugation and the medium was concentrated approximately 30-fold by ultrafiltration.

C. Purification of BACE

The expressed BACE protein was purified by affinity chromatography on nickel agarose resin. Initially, the concentrated medium containing the expressed BACE protein was dialysed overnight against 50mM sodium phosphate pH 8.0, 50mM sodium acetate, 300mM NaCl and 10ml Ni-NTA agarose resin (Qiagen) and equilibrated in the above buffer. Imidazole (Sigma) was added to a final concentration of 5mM, Pefabloc (Roche Molecular Biochemicals, Lewes, UK) was

added to 0.1g/L and the sample was mixed gently overnight at 4°C. The nickel agarose resin was then loaded onto an empty column and washed with 50mM sodium phosphate pH 8.0, 300mM NaCl until the absorption at 280 nm reached the baseline level of the above-mentioned buffer. The column was then washed with 4 column volumes of 50mM sodium phosphate pH 8.0, 50mM NaCl, 15mM imidazole. The BACE protein was then eluted with a linear imidazole concentration gradient, five column volumes in size, from 50mM sodium phosphate pH 8.0, 50mM NaCl to 50mM sodium phosphate pH 8.0, 50mM NaCl, 300mM imidazole, typically resulting in an absorption peak at 280nm, corresponding to the BACE protein and other co-purified contaminating proteins.

After Nickel chromatography the BACE protein was purified by anion exchange chromatography, fractions corresponding to the BACE protein containing the peak were buffer exchanged on a XK-50 column (Amersham Pharmacia Biotech) containing 200 ml sephacryl S-200, into 25 mM Tris pH 8.1, 5mM NaCl (Anion loading buffer) and then loaded onto a Resource Q anion exchange column (Amersham Pharmacia Biotech). The protein was eluted with a 35 column volume linear salt gradient from 100% loading buffer to 100% elution buffer (25mM Tris pH8.1, 400mM NaCl). Fractions were pooled based on analysis by SDS-PAGE.

The pooled fractions were dialysed against HIC loading buffer: 50mM Tris pH 8.1, 50mM NaCl, 0.9 M (NH₄)₂SO₄. The final sample was then loaded onto a HIC column (Source PHE, Amersham Pharmacia Biotech) equilibrated with HIC loading buffer, and washed to a stable baseline with loading buffer. The differentially processed forms of the BACE generated by proteolytic activity were eluted as separate peaks using a 35 column volume gradient from loading buffer to 50mM Tris pH 8.1, 50mM NaCl.

Peak fractions containing the required form of BACE protein were pooled based on analysis by SDS-PAGE and dialysed against 50mM HEPES pH 8.0, 100mM NaCl, 1Mm DTT.

The dialysed sample was concentrated to a 12ml volume and loaded immediately onto a Sephacryl S-200 column (Amersham Pharmacia Biotech) pre-equilibrated with 50mM HEPES pH 8.0, 100mM NaCl, 1 Mm DTT and stored at 4°C after elution.

The purified BACE eluted from the size exclusion column at the position expected for monomeric protein and was monodisperse when subjected to dynamic light scattering. SDS-PAGE showed the representative samples after the different column steps is shown in Figure 5.

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EXAMPLE 2: Crystallization of BACE

A. Crystallization

Crystals of BACE were grown by the hanging drop vapor diffusion method, in which 1µl of protein solution and 1µl of well solution (100mM Tri-sodium citrate, pH 5.8, 200mM ammonium iodide and 18-20% PEG monomethyl ether, 5K) were placed on a cover slip and equilibrated over 1ml of well solution at 20°C. The protein concentration was 5mg/ml in 50mM HEPES, pH 8.0, 150mM NaCl, 1mM DTT. Small prismatic crystals appeared after two days and grew to a maximum size of 0.2mm x 0.1mm x 0.1mm after two weeks. (Figures 3A and B).

Crystals of BACE complexed with OM99-2 (Ghosh et al., 2000) were grown using a similar method. BACE, at a concentration of 0.2mg/ml was mixed with an excess of inhibitor and kept at 4°C for 1 hour. The BACE protein was then concentrated to 5mg/ml using a centricon column with a molecular weight cutoff of 10000, and the crystallization drops set up as before. Crystals with the same morphology as the uncomplexed enzyme appeared after two days and grew to a maximum size of 0.25mm x 0.1mm x 0.1mm.

Both BACE with no inhibitor and BACE in the presence of OM99-2 formed crystals belonging to space group C2. The cell dimensions for the crystals grown in the presence of OM99-2 (Figure 3A) were a=236.63Å, b= 105.02Å, c=62.59Å and β = 101.32°, and the asymmetric unit of the crystal contained 3 copies of BACE. The cell dimensions for the crystals grown in the absence of any inhibitor (Figure 3B) were a=238.3Å, b=107.4Å, c=60.4Å, b=101.89°.

Apo-Soaked Crystal Experimental: Crystals of BACE, grown in the absence of inhibitor as previously described were soaked in a solution of inhibitor for 1 hour. The inhibitor was previously dissolved in DMSO to a concentration of 10 mM and then diluted 1 in 10 in the well solution as previously described. 20 microliters of this was placed in a microbridge, and an apo BACE crystal added to it. The microbridge was sealed and incubated for 3.5 hours.

B. Data collection and processing

The structure of BACE as a complex with OM99-2 was solved to 2.6Å using the method of molecular replacement. Data was collected at 100K on crystals frozen in a solution containing a suitable cryoprotectant. The cryoprotectant solution consisted of 100mM Tri-sodium citrate, pH 5.8, 200mM ammonium iodide, 15% PEG monomethyl ether 5K, and 20% PEG 400. The crystal was immersed in the cryoprotectant solution for 30 seconds prior to freezing in liquid nitrogen for the purposes of storage. Data was collected to 2.6Å on beamline ID14-2 at the European

Synchrotron Radiation Facility using a MARCCD detector, with a wavelength of 0.934A and processed using D*trek (Pflugrath, J., 1999). The dataset was scaled using SCALA and the intensities converted to structure factors using TRUNCATE, from the CCP4 suite of programs (Collaborative Computing Project, 1994). Statistics for the processed data are listed in Table 1.

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TABLE 1: Data collection statistics for BACE crystallized as a complex with OM99-2.

| | 2.6Å |
|--------------|-------|
| Resolution | 2.011 |
| Mosaicity | 0.8° |
| Completeness | 95.4% |
| Multiplicity | 1.96 |
| Rmerge | 0.087 |

This table shows that the experimental data used to solve the structure of the BACE/OM99-2 complex was of good quality and sufficient completeness to enable a reliable structure to be derived from it.

Apo-Crystal Experimental: The soaked crystal was then removed, dipped in a solution containing a cryoprotectant mixed with the inhibitor in DMSO, in the same proportions as previously (100 mM Tri-sodium citrate, pH 5.8, 200 mM ammonium iodide, 15% PEG monomethyl ether 5K and 20% PEG 400). The crystal was then frozen as for the OM99-2 crystals and data collected. Data was collected on station ID14-1 at the ESRF using an ADSC detector.

C. Structure Determination and Refinement

The structure of the BACE/OM99-2 complex was solved by molecular replacement using the program AMORE (Navaza, 1994). The molecular replacement solution was not as straightforward application of AMORE. Rather, it involved the use of CCP4, the programs POLARRFN and RFCORR, as well as inventive effort, e.g., to so use this combination and especially to so use RFCORR (Collaborative Computing Project, 1994). The search model was the A chain of 1FKN (Hong et al. 2000) taken from the pdb database (1FKN.pdb); a search radius of 35Å and a resolution range of 8.0-3.0Å being used to give a solution with an Rfactor of 0.38 and a

correlation coefficient of 0.714. This solution was used as a starting point for refinement using the program REFMAC5, also from the CCP4 suite of programs (Collaborative Computing Project, 1994). The inhibitor, OM99-2 was absent from the initial model, and convincing electron density in the active site of all three copies of BACE was observed in difference Fourier maps. This provided confirmation that the solution to the molecular replacement was correct. Cycles of refinement of the structure were alternated with manual rebuilding of the model using QUANTA (1994, San Diego, CA: Molecular Simulations). The N- and C- termini of the molecule were rebuilt, asparagine residues 153, 172, 223 and 354 were remodeled as glutamine residues. The inhibitor molecule was built into the electron density with QUANTA (1994, San Diego, CA: Molecular Simulations), and finally the water molecules were added using DenInt (Astex internal software library). Refinement statistics are shown in Table 2A.

Data collected with apo crystals soaked with inhibitor were processed using D*Trek (Pflugrath, J., 1999), and the intensities converted to structure factors using TRUNCATE, from the CCP4 suite of programs (Collaborative Computing Project, 1994).

The space group of these crystals has changed from the apo form (space group C2) to P2₁ with cell dimensions a=62.8, b=106.8Å, c=227.9Å and β =93.63°. The statistics are given in Table 2B below

The structure of the soaked BACE/inhibitor complex was solved by molecular replacement using the programs AMORE (Navaza, 1994). The search model was a monomer from the BACE/OM99-2 structure. A search radius of 35 Å and a resolution range of 12 – 4Å gave a solution with and Rfactor of 0.421 and a correlation coefficient of 0.638. There are 6 monomers in the asymmetric unit. This solution was used as a starting point for refinement using the programs CNX (1999, San Diego, CA: Molecular Simulations) and BUSTER (Bricogne, 1993, Acta Cryst. D49, 37-60). The final refinement statistics are given in Table 2C below.

TABLE 2A: Final refinement statistics for The C2 BACE/OM99-2 complex.

| Rwork | 0.231 | |
|--|--------------------|-------|
| Rfree | 0.312 | |
| RMS bond deviation from ideality | 0.022Å | |
| RMS bond angle deviation from ideality | 2.4° | |
| Average Bfactor for structure | 53.4Å ² | · |

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This data indicates that the final structure is of good quality, the Rfactors indicating that the refined model has a good agreement with the experimental data. The RMS deviations from ideality indicate that the geometry of the model is good and in agreement with previous data.

TABLE 2B: Statistics for P2₁ BACE/inhibitor complex

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| Resolution | 3.0 Å |
|--------------|-------|
| Mosaicity | 0.45 |
| Completeness | 98% |
| Multiplicity | 2.3 |
| Rmerge | 13.8% |

The statistics show the space group has changed from the apo-BACE form (space group C2) to P2₁ with cell dimensions a=62.8, b=106.8Å, c=227.9Å and β=93.63°

TABLE 2C: Final refinement statistics for P2₁ BACE/inhibitor complex.

| Rwork | 30.3% | · |
|--|---------|---|
| Rfree | 34.5% | |
| RMS bond deviation from ideality | 0.015 Å | |
| RMS bond angle deviation from ideality | 1.027° | |
| Average Bfactor for structure | 35.6 Å | |

RESULTS AND DISCUSSION

The final model of the C2 crystal structure of BACE/OM99-2 contained 1161 residues in 3 protein molecules, 3 copies of OM99-2 and 183 ordered water molecules, an Rfactor of 0.231 and a free Rfactor of 0.312. The asymmetric unit contained 3 copies of the BACE molecule (Figures 4A and B), A, B and C, two of which, B and C, form a dimer related by a non-crystallographic two-fold axis. Molecule A forms a similar dimer with its crystallographically related molecule A in an adjacent asymmetric unit. The positions of residues –2 to 385 of all three independent molecules are well defined by the electron density. There is no evidence of density beyond serine –2 for any of the molecules, and the N-terminus of molecules A and C interact with OD1 of asparagine 98 in symmetry related molecules B and A respectively. The N-terminus of molecule B is in a region of solvent. This lack of electron density for all three molecules indicates that the other residues from the N-terminus have no ordered structure. The electron density at the C-terminus ends with residue Asn 385, with no evidence for further terminal residues for the His-tag.

The bilobal structure of individual molecules of BACE as solved in the C2 crystal form, is essentially the same as that of memapsin 2 as solved in the P2₁ crystal form. The interactions made by the specific mutations are shown in Table 3. These include the N and C-terminus and the Asn → Gln mutations in each of the three independent units. The mutation of Asn111 to Gln111 appears to be important in the formation of the crystals in that Gln111 of molecule B lies close to the crystallographic two-fold axis and interacts with the symmetry related B:111. Difference electron density was initially seen for OM99-2 in all three molecules, and the inhibitor molecule was fitted to this. Its position was well defined from P4 to P4' for molecules A and C P4' was less well defined in molecule B. The active site is open to solvent for molecules B and C, but that of molecule A is partially occluded (close to P4') by a symmetry related molecule C.

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TABLE 3: Interactions made by mutated residues in BACE. Monomers AB and C are described in column 1 and the residues with which they interact in column 2.

| Mutated or different residue (from | Interactions formed by mutated or different |
|------------------------------------|---|
| Tang sequence) | residue. |
| A:92 | B:142, a crystallographic symmetry related lysine |
| A:111 | No direct interactions |
| A:162 | No direct interactions |
| A:293 | No direct interactions |
| B:92 | No direct interactions |
| B:111 | B:111 symmetry related glutamine, lies on 2-fold |
| B:162 | Close to crystallographic symmetry axis, but no |
| | direct interactions |
| B:293 | Points towards solvent channel |
| C:92 | A:142 a crystallographic symmetry related lysine |
| C:111 | No direct interactions |
| C:162 | No direct interactions |
| C:293 | No direct interactions |
| A:Nterm | Nterm makes interaction with symmetry related |
| | OD1 of Asn98B |
| B:Nterm | Nothing beyond residue ser-2 |
| C:Nterm | N-term makes interaction with symmetry related |
| | OD1 of Asn98A |
| A:Cterm | No interactions |
| B:Cterm | No interactions |
| C:Cterm | No interactions. |

This table shows that most of the mutations made to the BACE enzyme are at positions which do not affect the crystal packing. The major exception is in the case of residue B111, which is shown to interact across the crystallographic two-fold axis with its symmetry related molecule.

5 TABLE 4: Comparison of Tang/Hong structure with present invention.

| Measurement | Tang/Hong | Present Invention |
|------------------------------|---------------------------------|-------------------------------|
| Inhibitor OM99-2 | Crystallized in presence of | Crystallized in presence and |
| | inhibitor OM99-2 | absence of OM99-2. |
| Crystallisation conditions | 5mg/ml protein, 5-fold molar | 6mg/ml protein, excess |
| 0.,0 | excess of OM99-2 | OM99-2, 0.2M ammonium |
| | 0.2M ammonium sulphate,22.5% | iodide, 20% PEGMME5K, |
| | PEG8K, 0.1M Na-cacodylate, | 0.1M tri-sodium citrate, pH |
| | pH 7.4 | 5.6-5.8 |
| Space Group | P2 ₁ | C2 |
| Cell dimensions(Å) | a=53.7,b=85.9,109.2,beta=101.4° | a=236.6,b=105.0,c=62.59, |
| | | beta=101.3° |
| Resolution | 1.9Å | 2.6Å |
| pH of crystallization | 7.4 | 5.8 |
| Molecules in asymmetric | 2 | 3 |
| unit | | |
| N-terminus | -28p | -33p |
| C-terminus | No His-tag | His-tag |
| Mutations | None known | Asn→Gln (glycosylation |
| | | sites) |
| Dimer interface | Around N209 | Same dimer interface |
| B:111 environment | solvent exposed | interact across 2-fold axis. |
| Accessibility of active site | Both molecules accessible | 1 accessible, 1 inaccessible, |
| | | 1 partly accessible |
| OM99-2 binding mode | As described in Science, 2000 | Binding modes similar, but |
| | 290 150-153 | P4' is more ordered. |

This further demonstrates that the present invention is novel, nonobvious and inventive over the Tang PCT publications and the Hong Science article.

The following Table 5 provides atomic co-ordinates of BACE.

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```
Table 5: Atomic co-ordinates.
                                                      XX-XXX-XX
                                                                  XXXX
              ----
    HEADER
    COMPND
             3
    REMARK
             3 REFINEMENT.
    REMARK
                            : REFMAC 5.0
                 PROGRAM
10
    REMARK
    REMARK
    REMARK
                  REFINEMENT TARGET : MAXIMUM LIKELIHOOD
    REMARK 3
            3 DATA USED IN REFINEMENT.
    -REMARK
             3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.60
    REMARK
                 RESOLUTION RANGE LOW (ANGSTROMS): 119.52
    REMARK
                 DATA CUTOFF (SIGMA(F)): NONE
    REMARK
             3 COMPLETENESS FOR RANGE (%): 93.40
     REMARK
             3 NUMBER OF REFLECTIONS
20 REMARK
     REMARK
             3 FIT TO DATA USED IN REFINEMENT.
     REMARK
            3 CROSS-VALIDATION METHOD : THROUGHOUT
3 FREE R VALUE TEST SET SELECTION : RANDOM
3 R VALUE (WORKING + TEST SET) : 0.23480
     REMARK
     REMARK
25
     REMARK
                            (WORKING SET) : 0.23064
            3 R VALUE
     REMARK
                                              : 0.31230
                 FREE R VALUE
     REMARK
                 FREE R VALUE TEST SET SIZE (%): 5.1
FREE R VALUE TEST SET COUNT : 2184
     REMARK
     REMARK
30
     REMARK
                 FIT IN THE HIGHEST RESOLUTION BIN.
     REMARK
                                                            20
                  TOTAL NUMBER OF BINS USED
     REMARK
                                                           2.601
                  BIN RESOLUTION RANGE HIGH
     REMARK
                 BIN RESOLUTION RANGE LOW
                                                           2.668
     REMARK
              3 REFLECTION IN BIN (WORKING SET) :
3 BIN R VALUE (WORKING SET) :
                                                           2799.
35
     REMARK
                                                           0.282
                  BIN R VALUE
     REMARK
                  BIN FREE R VALUE SET COUNT
                                                           145
     REMARK 3
                                                           0.403
                  BIN FREE R VALUE
     REMARK
     REMARK
                 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
     REMARK 3
40
                                         : 9531
             3
                  ALL ATOMS
     REMARK
     REMARK
              3 B VALUES.
3 FROM WILSON PLOT (A**2): NULL
3 MEAN B VALUE (OVERALL, A**2): 50.041
              3 B VALUES.
     REMARK
     REMARK
      REMARK
              3 OVERALL ANISOTROPIC B VALUE.
     REMARK
      REMARK 3
                 B11 (A**2) : -4.02
                  B22 (A**2) :
                                   -0.68
      REMARK 3
                   B33 (A**2) :
                                  4.60
      REMARK 3
                 B12 (A**2) : 0.00
      REMARK 3
 50
                   B13 (A**2) :
                                   -0.24
      REMARK 3
                                  0.00
                   B23 (A**2) :
      REMARK
             3 -
      REMARK 3
      REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.
                                                                   (A): 1.142
                  ESU BASED ON R VALUE
      REMARK 3
 55
                                                                   (A):
                                                                          0.408
                  ESU BASED ON FREE R VALUE
              3
      REMARK
                                                                        0.512
                  ESU BASED ON MAXIMUM LIKELIHOOD
                                                                   (A):
      REMARK
                  ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 23.746
      REMARK
      REMARK
              3 CORRELATION COEFFICIENTS.
 60
      REMARK
```

PCT/GB02/03461

```
CORRELATION COEFFICIENT FO-FC
5
    REMARK . 3
                 CORRELATION COEFFICIENT FO-FC FREE:
    REMARK
            . 3
    REMARK
             3
                                                                         WEIGHT
                                                                 RMS
                                                        COUNT
                 RMS DEVIATIONS FROM IDEAL VALUES
    REMARK
              3
                                                    (A): 9582; 0.022; 0.021
                  BOND LENGTHS REFINED ATOMS
    REMARK
                                                    (A): 8445; 0.001; 0.020
                 BOND LENGTHS OTHERS
              3
10
    REMARK
                                              (DEGREES): 13011; 2.356; 1.945
                  BOND ANGLES REFINED ATOMS
    REMARK
              3
                                              (DEGREES): 19641; 0.973; 3.000
                  BOND ANGLES OTHERS
    REMARK
              3
                                              (DEGREES): 1173; 6.207; 3.000
                  TORSION ANGLES, PERIOD 1
    REMARK
              3
                                              (DEGREES): 1607;21.762;15.000
                  TORSION ANGLES, PERIOD 3
     REMARK
                                                 (A**3): 1422; 0.121; 0.200
                  CHIRAL-CENTER RESTRAINTS
15
   REMARK
                                                    (A): 10704; 0.003; 0.020
                  GENERAL PLANES REFINED ATOMS
     REMARK
                                                    (A): 2010; 0.001; 0.020
                  GENERAL PLANES OTHERS
     REMARK
              3
                  NON-BONDED CONTACTS REFINED ATOMS (A): 2679; 0.339; 0.300
     REMARK
              3
                                                    (A): 9125; 0.264; 0.300
                  NON-BONDED CONTACTS OTHERS
              3
     REMARK
                                                            3; 0.093; 0.500
                                                    (A):
                  NON-BONDED TORSION OTHERS
              3
20
     REMARK
                                                           834 ; 0.226 ; 0.500
                  H-BOND (X...Y) REFINED ATOMS
                                                    (A):
     REMARK
                                                            35 ; 0.161 ; 0.500
                  H-BOND (X...Y) OTHERS
                                                    (A):
     REMARK
                                                            20 ; 0.299 ; 0.300
                                                    (A):
                  SYMMETRY VDW REFINED ATOMS
     REMARK
                                                    (A):
                                                            62 ; 0.395 ; 0.300
                  SYMMETRY VDW OTHERS
     REMARK
                                                            10 ; 0.351 ; 0.500
                  SYMMETRY H-BOND REFINED ATOMS
                                                    (A):
     REMARK
                                                             2 ; 0.229 ; 0.500
                  SYMMETRY H-BOND OTHERS
                                                    (A):
     REMARK
     REMARK
                 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                                          COUNT
                                                                 RMS
     REMARK
                  MAIN-CHAIN BOND REFINED ATOMS (A**2): 5889; 3.453; 5.000
     REMARK
                                                          9501 ; 5.002 ; 6.000
                  MAIN-CHAIN ANGLE REFINED ATOMS (A**2):
30
     REMARK
                                                          3693 ; 4.504 ; 6.000
                  SIDE-CHAIN BOND REFINED ATOMS (A**2):
     REMARK
                  SIDE-CHAIN ANGLE REFINED ATOMS (A**2):
                                                          3510 ; 6.644 ; 7.500
     REMARK
     REMARK
                 NCS RESTRAINTS STATISTICS
     REMARK
                  NUMBER OF NCS GROUPS : NULL
35
     REMARK
              3
     REMARK
              3
     REMARK
                 TLS DETAILS
              3
     REMARK
                  NUMBER OF TLS GROUPS : NULL
     REMARK
40
     REMARK
     REMARK
                 BULK SOLVENT MODELLING.
     REMARK
                   METHOD USED : BABINET MODEL WITH MASK
     REMARK
                   PARAMETERS FOR MASK CALCULATION
              3
     REMARK
                   VDW PROBE RADIUS : 1.40
 45
     REMARK
               3
                                      :
                                          0.80
                   ION PROBE RADIUS
      REMARK
               3
                   SHRINKAGE RADIUS
                                         0.80
      REMARK
      REMARK
                  OTHER REFINEMENT REMARKS:
      REMARK
               3 HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
 50
      REMARK
               3
      REMARK
                                                             0.00
                                      23
                               PRO A
      CISPEP
               1 SER A
                                                             0.00
                               PRO A 129
               2 ARG A 128
      CISPEP
                                                             0.00
                               PRO A 373
               3 GLY A 372
      CISPEP
                               CYS A
                                      359
               1 CYS A 155
 55
      SSBOND
                               CYS A
                                      382
      SSBOND.
               2 CYS A 217
               3 CYS A 269
                               CYS A
                                      319
      SSBOND
                                                             0.00
               4 SER B
                        22
                               PRO B
                                       23
      CISPEP
                                                             0.00
                               PRO B
                                      129
      CISPEP
               5 ARG B 128
                                                             0.00
                               PRO B
                                      373
               6 GLY B
                        372
      CISPEP
 60
                               CYS B
                                      359
               4 CYS B
                        155
      SSBOND
```

```
217
                                CYS B
                                       382
5
     SSBOND
              5 CYS B
              6 CYS B
                        269
                                CYS B
                                       319
     SSBOND
                         22
                                PRO C
                                       . 23
                                                                0.00
              7 SER C
     CISPEP
                                                                0.00
     CISPEP
              8 ARG C
                        128
                                PRO C
                                       129
                                                                0.00
                                PRO C
                                       373
                GLY C
                        372
     CISPEP
              7 CYS C
                                CYS C
                                       359
10
     SSBOND
                        155
              8 CYS C
                        217
                                CYS C
                                       382
     SSBOND
                                CYS C
     SSBOND
              9 CYS C
                        269
                                       319
                                  62.590 90.00 101.32 90.00 C 1 2 1
             236.630 105.020
     CRYST1
                            0.000000
                                       0.000846
                                                        0.00000
                 0.004226
     SCALE1
                                                        0.00000
15
                 0.000000
                            0.009522
                                       0.000000
     SCALE2
                                                        0:00000
                 0.000000
                            0.000000
                                      0.016294
     SCALE3
                                                        12.324 1.00 34.66
                       SER A
                                       17.150 -22.147
     MOTA
               1 N
                              -2
                       SER A
                              -2
                                       18.119 -22.435
                                                        11.206
                                                                 1.00 39.63
     · MOTA
               3 CA
                              -2
                                       17.523 -22.274
                                                                 1.00 43.29
               5
                 CB
                       SER A
                                                         9.764
     MOTA
                                                                                        0
                                       17.135 -20.963
                                                         9.336
                                                                 1.00 46.72
20
               8
                  OG
                       SER A
                              -2
     MOTA
                                                                                        C
              10
                       SER A
                              -2
                                       19.507 -21.833
                                                        11.428
                                                                 1.00 41.17
     MOTA
                  С
                                                                 1.00 58.68
                                       20.479 -22.532
                                                        11.183
                                                                                        0
     MOTA
              11
                   0
                       SER A
                              -2
                                       19.649 -20.573
                                                        11.846
                                                                 1.00 44.17
                                                                                        N
     MOTA
              14
                   N
                       PHE 'A
                              -1
                                       20.910 -20.078
                                                                 1.00 38.71
                                                        12.436
     MOTA
              16
                   CA
                       PHE A
                              -1
                                       21.526 -19.134
25
                       PHE A
                                                        11.408
                                                                1.00 40.94
                   CB
                              -1
     ATOM
              18
                                                                 1.00 34.80
                                                                                        C
                       PHE A
                                       21.855 -19.846
                                                        10.113
              21
                   CG
                               -1
     ATOM
                                                                                        C
              22
                                       20.860 -20.099
                                                                 1.00 33.03
                   CD1 PHE A
                                                         9.181
                               -1
     ATOM
                                                                                        С
                                       21.162 -20.772
                                                         8.020
                                                                 1.00 44.01
              24
                   CE1 PHE A
                               -1
     ATOM
                                                                                        С
                                       22.473 -21.212
                                                         7.783
                                                                 1.00 40.67
     ATOM
              26
                   CZ
                       PHE A
                              -1
                                                         8.704
                                                                                        С
                                       23.455 -20.971
                                                                 1.00 41.60
30
     ATOM
               28
                   CE2 PHE A
                               -1
                                       23.146 -20.297
                                                         9.864
                                                                 1.00 41.30
                                                                                        С
                   CD2 PHE A
     ATOM
               30
                               -1
                                                                                        С
               32
                   С
                       PHE A
                               -1
                                       20.809 -19.447
                                                        13.873
                                                                 1.00 48.71
     ATOM
                                       21.220 -18.282
                                                        14.082
                                                                 1.00 52.36
                                                                                        0
               33
                   0
                       PHE A
                               -1
     MOTA
                       VAL A
                                       20.309 -20.241
                                                        14.848
                                                                 1.00 50.55
                                                                                        N
     ATOM
              34
                   N
                                0
                                                                                        C
35
               36
                   CA
                       VAL A
                                0
                                       19.944 -19.816
                                                        16.243
                                                                 1.00 50.67
     ATOM
                                       19.252 -20.960
                                                                                        C
                                                        17.037
                                                                 1.00 54.02
     ATOM
               38
                   CB
                       VAL A
                                0
                                                                                        С
                                       17.851 -21.180
                                                        16.565
                                                                 1.00 59.81
     MOTA
               40
                   CG1 VAL A
                                O
                   CG2 VAL A
                                       20.016 -22.211
                                                        16.926
                                                                 1.00 54.45
                                                                                        С
               44
                                0
     ATOM
                                       21.047 -19.362
                                                                 1.00 47.63
                                                                                        С
               48
                   C
                       VAL A
                                0
                                                        17.171
     MOTA
                                                                                        O
40
                                       20.864 -18.642
                                                        18.174
                                                                 1.00 47.19
               49
                   0
                       VAL A
                                0
     MOTA
                                       22.195 -19.867
                                                        16.855
                                                                 1.00 47.53
                                                                                        N
               50
                   N
                       GLU A
                                1
     ATOM
                                                                 1.00 45.35
     ATOM
               52
                   CA
                       GLU A
                                1
                                       23.444 -19.407
                                                        17.410
                                       24.489 -19.994
                                                        16.474
                                                                 1.00 46.47
               54
                   CB
                       GLU A
     MOTA
                                1
                                                                 1.00 37.41
               57
                   CG
                       GLU A
                                       23.893 -20.218
                                                        15.070
     ATOM
                                1
                                                                                        C
45
               60
                   CD
                       GLU A
                                1
                                       24.627 -21.224
                                                        14.257
                                                                 1.00 36.90
     MOTA
                                                                                        0
                   OE1 GLU A
                                       23.964 -21.926
                                                        13.487
                                                                 1.00 29.13
     MOTA
               61
                                1
                                                                                        0
               62
                   OE2 GLU A
                                       25.868 -21.304
                                                        14.382
                                                                 1.00 44.61
     MOTA
                                1
                       GLU A
                                       23.573 -17.933
                                                        17.273
                                                                 1.00 44.07
                                                                                        Ċ
     MOTA
               63
                   С
                                1
                                       23.950 -17.227
                                                                 1.00 47.47
                                                                                        0
     ATÓM
               64
                   0
                       GLU A
                                1
                                                        18.185
                                      23.211 -17.471
                                                        16.087
50
                       MET A
                                                                 1.00 48.56
     ATOM
               65
                   N.
                                2
                                       23.536 -16.135
                                                        15.628
                                                                 1.00 44.26
               67
                   CA
                       MET A
                                2
     ATOM
                   CB
                       MET A
                                       23.886 -16.271
                                                         14.156
                                                                 1.00 46.78
               69
                                2
     ATOM
                                                                                        С
                                      24.968 -17.287
                                                        13.979
               72
                   CG
                       MET A
                                2
                                                                 1.00 46.07
     MOTA
               75
                   SD
                       MET A
                                       25.968 -17.107
                                                         12.614
                                                                 1.00 44.85
                                2
     MOTA
                                                         11.580
                                                                                        С
55
               76
                   CE
                       MET A
                                2
                                        25.329 -18.379
                                                                 1.00 47.63
     MOTA
               80
                   С
                       MET A
                                2
                                        22.441 -15.143
                                                         15.782
                                                                 1.00 44.93
                                                                                        C
     MOTA
                                        22.694 -13.949
                                                        15.928
                                                                                        0
     MOTA
               81
                   0
                       MET A
                                2
                                                                 1.00 44.66
                       VAL A
                                        21.213 -15.640
                                                         15.739
                                                                                        N
               82
                   N
                                                                 1.00 44.93
                                3
     MOTA
               84
                   CA
                       VAL A
                                       20.054 -14.792
                                                         15.864
                                                                 1.00 42.74
                                                                                        С
                                3
     ATOM
                                       18.787 -15.658
                                                         15.886
60
     ATOM
               86
                   CB
                       VAL A
                                3
                                                                 1.00 41.67
                   CG1 VAL A
                                        17.725 -15.033
                                                         16.713
                                                                 1.00 37.90
               88
     MOTA
```

| 5 | MOTA | 92 | CG2 | VAL A | A 3 | } | 1 | 8.319 | -15.879 | 14.506 | 1.00 | 37.99 | | | С | |
|-----|--------|-----|-----|-------|--------------|----------|---|------------------|---------|--------|------|---------|---|---|-----|---|
| | ATOM | 96 | С | VAL A | | | 2 | 20.178 | -14.009 | 17.153 | | 43.63 | | | C. | |
| | ATOM | 97 | 0 | VAL A | A 3 | 1 | 2 | 20.474 | -14.592 | 18.164 | 1.00 | 38.26 | | • | Q | |
| | ATOM | 98 | N | ASP F | A . 4 | ļ | 1 | 19.953 | -12.696 | 17.100 | 1.00 | 45.42 | | | N | |
| | ATOM | 100 | CA | ASP F | | Į | | | -11.823 | 18.267 | 1.00 | 45.76 | | | С | |
| 10 | ATOM | 102 | СВ | ASP A | | | | | -12.445 | 19.482 | 1.00 | 53.20 | | | С | |
| 10 | ATOM | 105 | CG | ASP F | | | | | -12.638 | 19.299 | | 65.48 | | | С | |
| | ATOM | 106 | | ASP F | | | | | -13.367 | 20.153 | | 74.58 | | | 0 | |
| | MOTA | 107 | | ASP A | | | | | -12.144 | 18.367 | | 62.82 | | | 0 | |
| • | ATOM | 108 | C | ASP F | | | | | -11.521 | 18.742 | | 45.27 | | | С | |
| 15 | ATOM | 109 | ò | ASP A | | | | | -11.253 | 19.923 | | 50.54 | | | 0 | |
| 13 | ATOM | 110 | N | ASN A | | | | | -11.539 | 17.888 | | 41.26 | | | N | |
| | ATOM | 112 | CA | ASN I | | , , | | | -11.339 | 18.387 | | 35.44 | | | C | |
| | ATOM | 114 | CB | ASN A | | | | | -12.331 | 17.728 | | 37.18 | | • | C | |
| • | | 117 | CG | ASN A | | , 5 | | | -12.137 | 16.262 | | 39.34 | | | C | |
| 20 | ATOM | 118 | | ASN A | | , 5 | | | -11.544 | 15.736 | | 38.77 | | | ō | |
| 20 | MOTA | • | | ASN A | | , 5 | | | -12.618 | 15.586 | | 35.75 | | | N | |
| | MOTA | 119 | | | | , 5 | | 23.811 24.387 | | 18.228 | | 38.11 | | | Ċ | |
| | ATOM | 122 | C | ASN A | | | | | | | | 37.36 | * | | ő | |
| | MOTA | 123 | 0 | ASN A | | - | | 25.585 | | | | 38.41 | | | N | |
| 05 | ATOM | 124 | N | LEU A | | | | 23.549 | | 17.833 | | 33.19 | | | C | |
| 25 | ATOM | 126 | CA | LEU A | | 5 | | 23.939 | | 17.679 | | 26.93 | | | C | |
| | MOTA | 128 | CB | LEU A | | <u>.</u> | | 23.468 | | 16.340 | | 27.79 | | | C | |
| | ATOM | 131 | CG | LEU A | | 5 . | | 24.086 | | 15.007 | | | | | C | |
| | MOTA | 133 | | LEU A | | 5 | | 23.717 | | 14.059 | | 27.07 | | • | | |
| | MOTA | 137 | | TEO 1 | | 5 | | 25.567 | | 14.998 | | 22.82 | | | C | |
| 30 | MOTA | 141 | С | LEU A | | 5 . | | 23.293 | | 18.756 | | 36.63 | | | C | |
| | ATOM | 142 | 0 | LEU A | | 6 | | 22.262 | | 19.284 | | 46.36 | | | 0 | |
| | ATOM | 143 | N | ARG A | | | | 23.875 | | 19.075 | | 41.26 | | | N | |
| ÷ | MOTA | 145 | CA | ARG A | | 7 | | 23.290 | | 20.038 | | 40.38 | | | C | |
| | MOTA | 147 | CB | ARG A | | 7 | | 23.833 | | 21.451 | | 44.61 | • | | C | |
| 35 | MOTA | 150 | CG | ARG A | | 7 | | 23.137 | | 22.209 | | 57.60 | | | C | |
| | MOTA | 153 | CD | ARG A | | 7 | | 23.680 | | 23.630 | | 65.11 | | | . C | |
| | MOTA | 156 | NE | ARG A | | 7 | | 25.141 | | 23.667 | | 76.98 | | | N | |
| | MOTA | 158 | CZ | ARG I | | 7 | | 25.947 | | 24.706 | | 82.43 | | | С | |
| | MOTA | 159 | NH1 | ARG I | | 7. | | 25.468 | | 25.845 | | 83.89 | | | N | |
| 40 | ATOM | 162 | NH2 | ARG I | A | 7 | | 27.256 | | 24.603 | | 82.28 | | | N | |
| | MOTA | 165 | С | ARG | A | 7 | | 23.627 | -3.196 | 19.506 | | 37.09 | | | С | |
| | MOTA | 166 | 0 | ARG I | A | 7 | | 24.329 | -3.119 | 18.506 | | 39.77 | | | 0 | |
| | MOTA | 167 | N | GLY : | A | В | | 23.139 | -2.136 | 20.139 | | 41.94 | • | | N | |
| | ATOM | 169 | CA | GLY 2 | Α | 8 | | 23.316 | -0.770 | 19.642 | 1.00 | 46.85 | | | С | |
| 45 | MOTA | 172 | ·C | GLY : | A ` | 8 | | 22.093 | -0.084 | 18.994 | 1.00 | 53.78 | | | С | |
| | MOTA | 173 | 0 | GLY : | A | 8 | | 20.926 | -0.485 | 19.254 | 1.00 | 49.83 | | | О | |
| | ATOM | 174 | N | LYS | A | 9 | | 22.345 | 0.968 | 18.169 | | 56.06 | | | N | |
| | MOTA | 176 | CA | LYS . | A . | 9 | | 21.272 | 1.585 | 17.372 | 1.00 | 58.92 | | | С | |
| | ATOM | 178 | CB | LYS | | 9 | | 20.312 | | 18.314 | 1.00 | 65.60 | | | С | |
| 50 | ATOM | 181 | CG | LYS . | | 9 | | 20.817 | 3.673 | 18.821 | 1.00 | 71.58 | | | С | |
| | ATOM | 184 | CD | LYS | | 9 | | 19.785 | | 19.712 | 1.00 | 76.80 | | | C | |
| | ATOM | 187 | CE. | LYS | | 9 | | 20.460 | | 20.645 | | 81.30 | | | C | |
| | ATOM | 190 | | LYS | | 9 | | 19.689 | | 21.898 | | 79.59 | | | N | , |
| | ATOM | 194 | C | LYS | | 9 . | | 21.662 | | 16.157 | | 57.10 | • | | ; c | |
| 55 | ATOM . | 195 | ò | LYS | | 9 | | 22.801 | | 15.996 | | 53.27 | | | Ö | |
| 55 | | 196 | Ń | SER | | | | 20.691 | | 15.312 | | 58.39 | • | | N | |
| | ATOM | 198 | CA | SER | | 0 | | 21.022 | | 14.153 | | 59.37 | | , | C | |
| | ATOM | 200 | CB | SER | | 0 | | 19.791 | | 13.417 | | 63.36 | • | | Ċ | |
| | ATOM | | OG | SER | | 0 | | 18.789 | | 14.345 | | 73.85 | | | Ö | |
| ۲۵. | MOTA | 203 | | | | 0 | | | | | | 61.22 | | | Ċ | |
| 60 | ATOM | 205 | C | SER | | 0 | | 21.724 | | 13.956 | | 64.24 | | | C | |
| | MOTA | 206 | 0 | SER | V 1 | J | | 22.617 | 5.434 | 10.000 | 1.00 | . 03.24 | | | • | |
| | | | | | | | | | | | | | | | | |

| 5. | ATOM | 207 | N | GLY A | A. | 11 | | 21.279 | 5.370 | 15.818 | 1.00 60.5 | | | N |
|-------------|--------------|------------|------------|-------|----|----------|---|------------------|------------------|------------------|------------------------|-----|---|--------|
| | ATOM | 209 | | GLY F | | 11 | | 21.807 | 6.519 | 16.499 | 1.00 49.9 | | | С |
| | ATOM | 212 | | GLY F | | 11 | | 23.308 | 6.455 | 16.511 | 1.00 53.4 | | | С |
| | MOTA | 213 | 0 | GLY F | 4 | 11 | | 23.952 | 7.390 | 16.020 | 1.00 42.2 | | | 0 |
| | ATOM | 214 | N | GLN A | Ą | 12 | | 23.864 | 5.357 | 17.052 | 1.00 51.8 | | | N |
| 10 | ATOM | 216 | CA | GLN A | A | 12 | | 25.313 | 5.236 | 17.206 | 1.00 51.0 | | | C |
| | ATOM | 218 | CB | GLN A | Ą | 12 | | 25.656 | 5.405 | 18.653 | 1.00 50.5 | | | С |
| | MOTA | 221 | CG | GLN A | A | 12 | | 25.254 | 6.733 | 19.190 | 1.00 53.2 | | | C |
| | ATOM | 224 | CD | GLN A | | 12 | | 25.455 | 6.803 | 20.686 | 1.00 53.3 | | | C |
| | MOTA | 225. | | GLN A | | 12 | | 25.155 | 5.827 | 21.393 | 1.00 51.6 | | | 0. |
| 15 | MOTA | 226 | NE2 | GLN A | | 12 | | 25.960 | 7.941 | 21.174 | 1.00 44.8 | | | N |
| | MOTA | 229 | С | GLN A | | 12 | | 25.939 | 3.922 | 16.774 | 1.00 54.0 | | | С |
| | MOTA | 230 | 0 | GLN A | | 12 | | 27.027 | 3.567 | 17.245 | 1.00 62.5 | | | 0 |
| | MOTA | 231 | N | GLY A | | 13 | | 25.264 | 3.200 | 15.897 | 1.00 49.5 | | | N |
| | MOTA | 233 | CA | GLY A | | 13 | | 25.763 | 1.941 | 15.424 | 1.00 43.8 | | | C |
| 20 ° | MOTA | 236 | .C | GLY A | | 13 | • | 25.250 | 0.639 | 16.051 | 1.00 44.9 | | | C |
| | MOTA | 237 | 0 | GLY A | | 13 | | 24.875 | 0.584 | 17.216 | 1.00 46.2 | | ٠ | O N |
| | MOTA | 238 | N | TYR A | | 14 | | 25.256 | -0.415 | 15.219 | 1.00 37.8 | | | C |
| | MOTA | 240 | CA | TYR A | | 14 | | 25.070 | -1.777 | 15.613 | 1.00 38.8 | | | C |
| | ATOM | 242 | CB | TYR A | | 14 | • | 24.228 | -2.432 | 14.566 | 1.00 43.5 | | | c |
| 25 | MOTA | 245 | CG | TYR A | | 14 | | 22.871 | -1.882 | 14.579 | 1.00 40.7 | | | C |
| | MOTA | 246 | | TYR A | | 14 | | 22.592 | -0.703 | 13.951 | 1.00 43.9 | | | C |
| | ATOM | 248 | | TYR I | | 14 | | 21.372 | -0.202 | 13.967 | 1.00 47.3 | | | Ċ |
| | MOTA | 250 | CZ | TYR I | | 14 | | 20.411 | -0.876 | 14.617 | 1.00 48.1 | | | 0 |
| | MOTA | 251 | ОН | TYR I | | 14 | | 19.178 | -0.405 | 14.638 | 1.00 49.4 | | | Ċ |
| 30 | ATOM | 253 | | TYR I | | 14 | | 20.659 | -2.045 | 15.246 | 1.00 45.9 1.00 39.2 | | | C |
| | MOTA | 255 | | TYR I | | 14 | | 21.883 | -2.532 | 15.224 15.658 | 1.00 39.2 | | | C |
| | MOTA | 257 | C | TYR | | 14 | • | 26.388 | -2.532 | | 1.00 33.2 | | | ŏ |
| | MOTA | 258 | 0 | TYR | | 14 | | 27.167 | -2.474 | 14.703 16.734 | 1.00 42.0 | | | N |
| 20 | MOTA | 259 | N | TYR | | 15 | | 26.610 | -3.291 -3.917 | 16.734 | 1.00 33.5 | | | c |
| 35 | ATOM | 261 | | TYR | | 15 | | 27.905 28.655 | -2.978 | 17.885 | 1.00 35.5 | | ٠ | C |
| | ATOM | 263 | CB | TYR | | 15 | | 28.090 | -2.976 | 19.303 | 1.00 38.0 | | | Ċ |
| | ATOM | 266 | CG | TYR . | | 15 15 | | 28.139 | -4.052 | 20.116 | 1.00 40.8 | | | C |
| | MOTA | 267 | | TYR. | | 15 | | 27.641 | -4.030 | 21.388 | 1.00 42.0 | | | C |
| 40 | MOTA | 269 | CZ | TYR . | | 15 | | 27.041 | -2.892 | 21.882 | 1.00 43.4 | | | Ċ |
| 40 | ATOM | 271 272 | OH | TYR | | 15 | | 26.593 | -2.912 | 23.176 | 1.00 40.4 | | | 0 |
| | MOTA | 274 | | TYR | | 15 | | 27.023 | -1.757 | 21.096 | 1.00 41.0 | | _ | С |
| | ATOM | 276 | | TYR | | 15 | | 27.522 | -1.787 | 19.816 | 1.00 38.3 | | | С |
| | MOTA MOTA | 278 | CDZ | TYR | | 15 | | 27.828 | -5.307 | 17.605 | 1.00 32. | | | С |
| 45 | ATOM | 279 | O. | TYR | | 15 | | 26.901 | -5.608 | 18.296 | 1.00 33. | | | 0 |
| 7.7 | ATOM | 280 | N. | VAL | | 16 | | 28.832 | -6.148 | 17.398 | 1.00 38. | | | N |
| | ATOM | 282 | CA | VAL | | 16 | | 28.763 | -7.554 | 17.781 | 1.00 36. | | | С |
| | MOTA | 284 | CB | VAL | | 16 | | 28.826 | | | | | | С |
| | | 286 | | VAL | | 16 | | 30.280 | -8.691 | 16.154 | 1.00 41. | | | С |
| 50 | MOTA | 290 | | VAL | | 16 | | 28.212 | -9.788 | 16.804 | 1.00 46. | | | C |
| 50 | MOTA | 294 | C | VAL | | 16 | | 29.993 | -7.861 | 18.579 | 1.00 37. | | | С |
| | MOTA | 295 | ŏ | VAL | | 16 | • | 30.995 | -7.188 | 18.388 | 1.00 37. | | | 0. |
| | ATOM | 296 | N | GLU | | 17 | | 29.898 | -8.861 | 19.461 | 1.00 32. | | | N |
| | ATOM | 298 | CA | GLU | | 17 | | 30.974 | -9.315 | 20.309 | 1.00 37. | | | Ċ |
| 55 | ATOM | 300 | CB | GLU | | 17 | | | -10.181 | 21.407 | 1.00 41. | | | С |
| 33 | ATOM | 303 | CG | GLU | | 17 | | | -10.529 | 22.669 | 1.00 41. | | | С |
| | ATOM | | | | | 17 | | | -11.380 | 23.676 | 1.00 53. | | | С |
| | ATOM | 306 307 | CD OE 1 | GLU | | 17 | | | -10.947 | 24.041 | 1.00 62. | | | ō |
| | MOTA | 308 | | GLU | | 17 | | | -12.484 | 24.114 | 1.00 47. | | | 0 |
| 60 | MOTA | 309 | C | GLU | | 17 | | | -10.162 | 19.538 | 1.00 39. | | | C |
| OU | ATOM ATOM | 310 | 0 | GLU | | 17 | | | -11.032 | 18.796 | 1.00 39. | | | Ō |
| | ATOM | 210 | J | GTO | А | 1, | | 51.057 | 11.002 | 20.,00 | | - • | | - |

| | • | | | | | · · | |
|-----------|--------------|------------|----------------|---------|------|--|------------|
| 5 | MOTA | 311 | N | MET A | 18 | 33.292 -9.925 19.711 1.00 44.75 | N |
| _ | MOTA | 313 | CA | MET A | 18 | 34.301 -10.791 19.082 1.00 41.54 | C |
| | ATOM | 315 | CB | MET A | 18 | 34.838 -10.160 17.802 1.00 41.81 | С |
| | MOTA | 318 | CG | MET A | 18 | 33.836 -9.447 16.939 1.00 41.86 | С |
| | ATOM | 321 | SD | MET A | 18 | 34.600 -8.833 15.425 1.00 50.01 | S |
| 10. | ATOM | 322 | CE | MET A | 18 | 35.054 -10.282 14.687 1.00 45.99 | С |
| | ATOM | 326 | С | MET A | 18 | 35.466 -10.864 20.038 1.00 43.74 | С |
| | ATOM | 327 | 0 | MET A | 18 | 35.596 -10.003 20.877 1.00 49.03 | 0 |
| | ATOM | 328 | N | THR A | 19 | 36.325 -11.868 19.937 1.00 45.52 | N |
| | ATOM | 330 | CA | THR A | 19 | 37.572 -11.813 20.698 1.00 45.53 | С |
| 15 | MOTA | 332 | CB | THR A | 19 | 37.747 -13.023 21.572 1.00 45.33 | С |
| | MOTA | 334 | OG1 | THR A | 19 | 38.226 -14.108 20.759 1.00 50.86 | 0 |
| | MOTA | 336 | CG2 | THR A | 19 | 36.463 -13.451 22.142 1.00 40.03 | C |
| | ATOM | 340 | С | THR A | 19 | 38.763 -11.893 19.814 1.00 45.19 | C |
| • | MOTA | 341 | O _j | THR A | 19 | 38.693 -12.560 18.785 1.00 47.81 | 0 |
| 20 | MOTA | 342 | N | VAL A | 20 | 39.865 -11.267 20.243 1.00 46.54 | N |
| | ATOM | 344 | CA | VAL A | 20 | 41.181 -11.385 19.556 1.00 46.08 | C |
| | ATOM | 346 | CB | VAL A | 20 | 41.657 -10.076 19.031 1.00 44.11 | C |
| | ATOM | 348 | | VAL A | 20 | 40.734 -9.589 17.998 1.00 51.93 | C |
| | ATOM | 352 | | VAL A | 20 | 41.687 -9.058 20.110 1.00 51.31 | C |
| 25 | ATOM | 356 | С | VAL A | 20 | 42.286 -11.858 20.490 1.00 48.60 | C |
| | ATOM | 357 | 0 | VAL A | 20 | 42.242 -11.643 21.715 1.00 49.22 | 0 |
| | MOTA | 358 | N | GLY A | 21 | 43.293 -12.505 19.944 1.00 49.38 | N |
| | ATOM | 360 | CA | GLY A | | 44.406 -12.881 20.791 1.00 51.59 | C |
| | ATOM | 363 | С | GLY A | | 44.282 -14.129 21.652 1.00 51.96 | C O |
| 30 | ATOM | 364 | 0 | GLY A | 21 | 43.216 -14.659 21.926 1.00 48.04 | N |
| | ATOM | 365 | N | SER A | 22 | 45.430 -14.604 22.087 1.00 51.50 45.462 -15.754 22.916 1.00 54.86 | C |
| • | MOTA | 367 | CA | SER A | 22 | | .C |
| | MOTA | 369 | CB | SER A | 22 | 46.238 -16.846 22.176 1.00 58.86 45.861 -16.909 20.794 1.00 60.35 | 0 |
| 25 | ATOM | | · OG | SER A | 22 | 46.156 -15.336 24.203 1.00 54.80 | č |
| 35 | MOTA | 374 | Ċ | SER A | | 47.217 -14.720 24.127 1.00 53.24 | ·ŏ |
| , | MOTA | 375 376 | O N | PRO A | 23 | 45.551 -15.566 25.378 1.00 54.99 | N |
| | ATOM ATOM | 377 | CA | PRO A | 23 | 44.141 -15.954 25.547 1.00 56.89 | С |
| | ATOM | 379 | СВ | PRO A | 23 | 43.945 -15.868 27.056 1.00 54.92 | С |
| 40 | ATOM | 382 | CG | PRO A | 23 | 45.075 -15.007 27.510 1.00 52.28 | С |
| 40 | ATOM | 385 | CD | PRO A | 23 | 46.218 -15.491 26.680 1.00 53.62 | С |
| | ATOM | 388 | C | PRO A | | 43.244 -14.889 24.943 1.00 56.89 | С |
| | ATOM | 389 | ō | PRO A | | 43.808 -13.858 24.604 1.00 57.85 | 0 |
| | ATOM | 390 | N | PRO A | | 41.931 -15.125 24.840 1.00 56.03 | N |
| 45 | ATOM | 391 | CA | PRO A | | 40.963 -14.220 24.217 1.00 52.69 | С |
| ••• | ATOM | 393 | СВ | PRO A | | 39.667 -15.023 24.276 1.00 52.70 | С |
| | ATOM | 396 | CG | PRO A | | 40.058 -16.369 24.440 1.00 55.89 | С |
| | MOTA | 399 | CD | PRO A | 24 | 41.259 -16.335 25.325 1.00 57.99 | С |
| | ATOM | 402 | | PRO A | | 40.697 -12.963 24.971 1.00 52.11 | С |
| 50° | ATOM | 403 | 0 1 | PRO A | 24 | 40.598 -13.028 26.170 1.00 56.31 | 0 |
| | ATOM | . 404 | N | GLN A | 25 | 40.558 -11.856 24.261 1.00 53.37 | N |
| | ATOM | 406 | CA | GLN A | 25 | 40.215 -10.568 24.839 1.00 54.86 | C. |
| | ATOM | 408 | СВ | GLN A | 25 | 41.290 -9.528 24.531 1.00 55.07 | C . |
| | ATOM | 411 | CG | GLN A | 25 | 42.627 -9.938 24.959 1.00 57.87 | . C |
| 55 | MOTA | 414 | CD | GLN A | 25 | 43.630 -8.867 24.743 1.00 56.36 | C |
| - | ATOM | 415 | OE1 | . GLN A | 25 | | 0 |
| | ATOM | 416 | NE2 | GLN A | 25 | | N |
| | ATOM | 419 | С | GLN A | . 25 | | С |
| | ATOM | 420 | 0 | GLN A | 25 | | 0 |
| 60 | ATOM | 421 | N | THR A | | | N |
| | MOTA | 423 | CA | THR A | 26 | 36.604 -9.597 24.436 1.00 50.69 | С |
| | | | | | | | |

| _ | 7 mov4 | 405 | СВ | THR | Δ | 26 | | 35.614 | -9.763 | 25.531 | 1.00 | 49.93 | | | 3 |
|----|--------------|------------|----------|-------|------|------|---|------------------|---------|---------|------|----------------|-------|-----|--------|
| 5 | MOTA | 425 | | THR | | 26 | | 35.404 | -11.164 | 25.799 | 1.00 | 53.75 | | | 0 |
| | MOTA | 427 | | THR | | 26 | | 34.308 | -9.246 | 25.060 | 1.00 | 46.30 | | - (| С |
| | ATOM | 429 | CGZ | THR | | 26 | | 36.575 | | 24.003 | 1.00 | 51.52 | | | С |
| | ATOM | 433 | | THR | | 26 | | 37.078 | -7.284 | 24.696 | | 59.94 | | 1 | 0 |
| 10 | ATOM | 434 | 0 | LEU | | 27 | | 35.982 | -7.856 | 22.858 | | 49.68 | | | N |
| 10 | MOTA | 435 | N | LEU | | 27 | | 35.858 | -6.476 | 22.412 | | 39.53 | | | С |
| | MOTA | 437 | CA | LEU | | 27 | | 37.066 | -6.094 | 21.592 | | 42.69 | | 4 | С |
| | MOTA | 439 | CB CG | LEU | | 27 | | 38.456 | -5.850 | 22.241 | | 44.73 | | | С |
| - | MOTA | 442 | | LEU | | 27 | | 39.404 | -5.301 | 21.192 | 1.00 | 42.23 | | | С |
| | MOTA | 444 | | LEU | | 27 | | 38.418 | -4.865 | 23.382 | | 44.45 | | | C T |
| 15 | ATOM | 448 | CDZ | LEU | | 27 | | 34.615 | -6.390 | 21.574 | 1.00 | 40.04 | | | С |
| | MOTA | 452 | | LEU | | 27 | | 34.313 | -7.319 | 20.821 | 1.00 | 40.69 | | • | 0 |
| | MOTA | 453 | O N | ASN | | 28 | | 33.859 | -5.305 | 21.704 | 1.00 | 43.27 | | | N |
| | ATOM | 454 | | ASN | | 28 | | 32.654 | -5.129 | 20.873 | 1.00 | 43.26 | | | С |
| 20 | MOTA | 456 | CA CB | ASN | | 28 | | 31.509 | -4.465 | 21.654 | 1.00 | 45.19 | | | С |
| 20 | ATOM | 458 | CG | ASN | | 28 | | 30.830 | -5.417 | 22.672 | 1.00 | 44.78 | | | С |
| | MOTA | 461 | | ASN | | 28 | | 30.936 | -5.234 | 23.888 | 1.00 | 47.19 | | | 0 |
| | MOTA | 462 | | ASN | | 28 | | 30.123 | -6.411 | 22.174 | | 42.58 | | | N |
| | MOTA | 463 466 | C | ASN | | 28 | | 33.018 | -4.308 | 19.633 | 1.00 | 45.28 | | | С |
| 25 | ATOM | 467 | Ö | ASN | | 28 | | 33.476 | -3.172 | 19.775 | 1.00 | 46.40 | ٠, | | 0 |
| 25 | MOTA | 468 | N | ILE | | 29 | | 32.795 | -4.911 | 18.450 | 1.00 | 46.88 | | | N |
| | MOTA | 470 | CA | ILE | | 29 | | 33.115 | -4.400 | 17.094 | 1.00 | 44.20 | | | C´ |
| | MOTA | 472 | CB | ILE | | 29 | | 33.690 | -5.561 | 16.303 | 1.00 | 43.47 | | | С |
| | MOTA | 474 | | ILE | | 29 | | 34.737 | -6.291 | 17.121 | | 43.10 | | | С |
| 20 | ATOM | 477 | | ILE | | 29 | | 35.870 | -5.421 | 17.574 | | 44.94 | • | | С |
| 30 | ATOM ATOM | 481 | | ILE | | 29 | | 34.248 | -5.079 | 14.973 | | 46.96 | | | С |
| | ATOM | 485 | C | ILE | | 29 | | 31.942 | -3.874 | 16.222 | | 41.20 | | | C |
| | ATOM | 486 | ō | ILE | | 29 | | 30.951 | -4.502 | 16.068 | | 36.51 | | | 0 |
| | MOTA | 487 | Ŋ | LEU | | 30 | | 32.084 | -2.715 | 15.617 | | 44.61 | | | N |
| 35 | ATOM | 489 | CA | LEU | | 30 | | 31.023 | | 14.783 | | 41.39 | | | C C |
| 55 | ATOM | 491 | СВ | LEU | A | 30 | | 31.284 | -0.684 | 14.562 | | 36.72 | • | | c |
| | ATOM | 494 | CG | LEU | A | 30 | | 30.022 | 0.080 | 14.326 | | 38.55 | | | C |
| | ATOM | 496 | CD1 | LEU | J A | 30 | | 29.865 | 1.229 | 15.255 | | 44.29 | | | c |
| | ATOM | 500 | CD2 | LEU | JA | 30 | | 30.137 | 0.569 | 12.982 | | 43.51 | | | c |
| 40 | ATOM | 504 | С | LEU | JA | 30 | | 30.885 | -2.911 | 13.455 | | 40.85 | | | o |
| | MOTA | 505 | 0 | LEC | JA | 30 | | 31.851 | -3.397 | 12.897 | | 45.44 | | | N |
| | ATOM | 506 | N | VAI | | 31 | | 29.662 | | 12.953 | | 43.56 42.56 | | | C |
| | MOTA | 508 | CA | IAV | | 31 | | . 29.362 | | 11.762 | | 44.28 | | | Č |
| , | ATOM | 510 | CB | | ЬA | 31 | | 28.116 | | | | 44.25 | | | Č |
| 45 | MOTA | 512 | | L VAI | | 31 | | 27.424 | | | | 48.98 | | | Ċ |
| | MOTA | 516 | | 2 VA1 | | 31 | | 28.472 | | | | 12.04 | | | Č |
| | · MOTA | 520 | C | | LА | | | 29.137 | | | | 46.43 | | | ō |
| | MOTA | 521 | O | | LΑ | | | 28.088 | | | | 38.37 | · · . | | N |
| | MOTA | . 522 | N | | PΑ | | | 30.113 | | | | 36.43 | | | C |
| 50 | ATOM | 524 | CA | | PΑ | | ٠ | 30.170 | | | | 0 41.59 | | | C |
| | MOTA | 526 | | | PΑ | | | 31.409 | | | | 0 46.08 | | | Ç |
| | MOTA | 529 | | | PΑ | | | 31.371 | | | | 0 58.39 | • | | 0 |
| | ATOM | 530 | | 1 AS | | | | 30.241 | | | • | 0 43.43 | | | 0 |
| | ATOM | 531 | | 2 AS | | | | 32.299 | | | | 0 36.03 | | | Ċ |
| 55 | ATOM | 532 | | AS | PA | 32 | | 30.308 | | | | 0 36.16 | | | 0 |
| | ATOM | 533 | | | | 32 | | 31.379 | | | | 0 35.12 | | • | N |
| | MOTA | 534 | | | | . 33 | | 29.238 | | | | 0 36.24 | • | | C |
| | ATOM | 536 | | | R A | | | 29.341 | | | | 0 40.04 | | | С |
| | MOTA | 538 | | | RA | | | 27.969 26.982 | | | | 0 44.25 | | | 0 |
| 60 | MOTA | 540 | | 1 TH | | | | | | | | 0 40.43 | | | С |
| | MOTA | 542 | . Ce | 2 TH | IK P | 33 | | 27.453 | 4.54 | , 5.575 | | | | | |

| 5 | ATOM | 546 | С | THR A | 33 | 29.829 | -1.581 | 4.301 | 1.00 33.30 | | | С |
|----|--------------|------------|--------|--------|----|------------------|------------------|----------------|--------------------------|---|---|--------|
| _ | ATOM | 547 | 0 | THR A | 33 | 29.893 | -1.701 | 3.085 | 1.00 35.29 | | • | 0 |
| | ATOM | 548 | N | GLY A | 34 | 30.177 | -0.493 | 4.946 | 1.00 31.75 | | | N |
| | ATOM | 550 | CA | GLY A | 34 | 30.601 | 0.715 | 4.245 | 1.00 36.33 | | | C |
| | ATOM | 553 | C | GLY A | 34 | 32.077 | 0.844 | 4.160 | 1.00 39.91 | | | С |
| 10 | ATOM | 554 | 0 | GLY A | 34 | 32.531 | 1.605 | 3.314 | 1.00 50.07 | | | 0 |
| | ATOM | 555 | N | SER A | 35 | 32.814 | 0.107 | 5.004 | 1.00 37.10 | | | N C |
| | ATOM | 557 | CA | SER A | 35 | 34.228 | 0.032 | 4.901 | 1.00 34.40 | | | |
| | ATOM | 559 | CB | SER A | 35 | 34.823 | 0.796 | 6.021 | 1.00 36.88 | | | C |
| | MOTA | . 562 | OG | SER A | 35 | 34.960 | -0.016 | 7.136 | 1.00 40.38 | | | O C |
| 15 | ATOM- | 564 | С | SER A | 35 | 34.785 | -1.406 | 4.922 | 1.00 37.08 | | | 0 |
| | ATOM | 565 | 0 | SER A | 35 | 34.045 | -2.332 | 5.176 | 1.00 32.07 1.00 37.61 | | | N |
| | MOTA | 566 | N | SER A | 36 | 36.104 | -1.546 | 4.668 | 1.00 37.61 | | | C |
| | MOTA | .568 | CA | SER A | 36 | 36.836 | -2.824 | 4.521 | 1.00 38.67 | | | Ċ |
| • | MOTA | .570 | CB | SER A | 36 | 37.384 | -2.903 | 3.110 | 1.00 39.32 | | | o · |
| 20 | MOTA | 573 | OG | SER A | 36 | 36.354 | -2.718 | 2.156 | 1.00 47.74 | | | c |
| | ATOM | 575 | С | SER A | 36 | 38.079 | -3.054 | 5.406 | 1.00 41.93 | | | ŏ |
| | MOTA | 576 | 0 | SER A | 36 | 38.978 | -3.850 | 5.074 | 1.00 42.44 | | | N |
| | MOTA | 577 | N | ASN A | 37 | 38.162 | -2.374 | 6.526 | 1.00 33.87 | | | C |
| • | MOTA | 579 | CA | ASN A | 37 | 39.299 | -2.563 | 7.336 | 1.00 36.25 | | | Ċ |
| 25 | MOTA | 581 | CB | ASN A | 37 | 39.969 | -1.216 | 7.505 | 1.00 35.23 | | | c |
| | MOTA | 584 | CG | ASN A | | 41.020 | -0.997 | 6.507 | 1.00 33.00 | | | Ö |
| | ATOM | 585 | | ASN A | 37 | 40.726 | -0.519 | 5.452 | 1.00 35.89 | | | N |
| | MOTA | 586 | | ASN A | 37 | 42.275 | ~1.379 | 6.819 8.679 | 1.00 30.50 | | | C. |
| | ATOM | 589 | С | ASN A | | 38.876 | -3.085 | 9.247 | 1.00 34.21 | | | ō |
| 30 | ATOM | 590 | 0 | ASN A | | 37.991 | -2.530 -4.157 | 9.184 | 1.00 34.21 | | | N |
| | MOTA | 591 | N | PHE A | | 39.478 | -4.137 -4.625 | 10.545 | 1.00 36.42 | | | C |
| • | MOTA | 593 | CA | PHE A | | 39.180 | -6.146 | 10.663 | 1.00 33.72 | • | | Ċ |
| | MOTA | 595 | CB | PHE A | | 39.256 | -6.678 | 12.040 | 1.00 43.00 | | | Ċ |
| ~~ | MOTA | 598 | CG | PHE A | | 38.886 39.713 | | 12.705 | 1.00 42.48 | | | c |
| 35 | ATOM | 599 | | PHE A | | 39.386 | -8.040 | 13.962 | 1.00 47.58 | | | С |
| | ATOM | 601 | | PHE A | | 38.233 | -7.661 | 14.586 | 1.00 42.81 | | | C |
| | MOTA | 603 | CZ | PHE A | | 37.394 | -6.785 | 13.954 | 1.00 49.46 | | | С |
| | MOTA | 605 | | PHE A | | 37.717 | -6.290 | 12.670 | 1.00 44.85 | | | С |
| 40 | ATOM | 607 | | PHE A | | 40.227 | -3.888 | 11.416 | 1.00 40.18 | | | С |
| 40 | MOTA | 609 | C O | PHE A | | 41.406 | -3.760 | 11.017 | 1.00 39.66 | | | 0 |
| | ATOM | 610 | N | ALA A | | 39.802 | -3.389 | 12.576 | 1.00 40.32 | | | -N |
| | MOTA | 611 613 | CA | ALA A | | 40.656 | | 13.403 | 1.00 40.28 | | | C |
| | MOTA | 615 | | ALA A | | 40.810 | | 12.739 | 1.00 40.18 | | | C |
| 45 | MOTA | 619 | CD | ALA A | | 40.020 | | 14.757 | 1.00 37.73 | | | С |
| 43 | ATOM . | 620 | o. | ALA A | | 38.787 | | 14.885 | 1.00 40.37 | | | 0 |
| | MOTA MOTA | 621 | N | VAL F | | 40.839 | | 15.764 | 1.00 38.68 | | | N |
| | ATOM | 623 | CA | VAL A | | 40.334 | | 17.117 | 1.00 39.39 | | | C |
| | ATOM | 625 | СВ | VAL: I | | 40.369 | -3.507 | 17.636 | 1.00 41.17 | | | С |
| 50 | ATOM | 627 | | VAL A | | 39.731 | | | 1.00 45.27 | | • | С |
| 50 | ATOM | 631 | | VAL A | | 41.722 | | 17.829 | 1.00 46.47 | | | . C |
| | ATOM | 635 | ,C | VAL A | | 41.080 | | 18.005 | 1.00 48.51 | | | С |
| | ATOM | 636 | ō | VAL 2 | | 42.175 | | 17.642 | 1.00 50.57 | • | | 0 |
| | | 637 | . N | GLY A | | 40.477 | | 19.152 | 1.00 47.86 | | | N |
| 55 | ATOM ATOM | 639 | CA | | | 41.073 | | 20.014 | 1.00 40.52 | | | · C |
| " | ATOM | 642 | C | GLY I | | 42.290 | | 20.595 | 1.00 44.67 | | | C |
| | ATOM | 643 | | GLY | | 42.140 | | 21.332 | 1.00 42.27 | | | 0 |
| | ATOM | 644 | | ALA I | | 43.500 | | 20.274 | 1.00 46.72 | | | N |
| | ATOM | | | ALA | | 44.724 | | 20.914 | | | | С |
| 60 | | 648 | | ALA | | 45.655 | | 19.886 | 1.00 42.07 | | | С |
| 00 | ATOM | 652 | | | | 45.444 | | 21.883 | 1.00 46.86 | | | С |
| | | | | | | | | | | | | |

| 5 | ATOM | 653 | 0 | ALA A | 4 | 2 | | 46.687 | 0.515 | 21.984 | 1.00 45.4 | 13 | | 0 |
|-----|------|-------|------|-------|-----|----------|---|---------|--------|---------|-----------|-----|----|----|
| ر | | 654 | N | ALA A | | | | 44.677 | 1.246 | 22.636 | 1.00 50.4 | 16 | | N |
| | MOTA | 656 | CA | ALA A | | | | 45.278 | 2.216 | 23.548 | 1.00 52. | 32 | | С |
| | ATOM | | CB | ALA A | | | | 46.320 | 3.073 | 22.854 | 1.00 48. | | | C |
| | ATOM | 658 | | | | | | 44.196 | 3.101 | 24.052 | 1.00 56. | | | С |
| 4.0 | ATOM | 662 | C | ALA A | | | | 43.186 | 3.315 | 23.380 | 1.00 57. | | | 0 |
| 10 | ATOM | 663 | 0 | ALA A | | | | 44.446 | 3.628 | 25.238 | 1.00 62. | | | N. |
| | MOTA | 664 | N | PRO A | | | | 43.510 | 4.492 | 25.962 | 1.00 59. | | | c |
| | ATOM | 665 | CA | PRO I | | | | | 5.093 | 27.053 | 1.00 62. | | | C |
| | ATOM | 667 | CB | PRO A | | | | 44.390 | | 26.603 | 1.00 66. | | • | C |
| | MOTA | 670 | CG | PRO A | | | | 45.835 | 4.754 | | 1.00 65. | | | Ċ |
| 15 | MOTA | 673 | CD | PRO I | | | | 45.696 | 3.411 | 26.003 | 1.00 59. | | - | C |
| | MOTA | 676 | ·C | PRO I | | 4 | | 42.905 | 5.606 | 25.132 | | | | o |
| | MOTA | 677 | 0 | PRO I | | 4 | | 43.553 | 6.133 | 24.218 | 1.00 55. | | | N |
| • | MOTA | 678 | N | HIS ! | A 4 | 5 | | 41.653 | 5.939 | 25.452 | 1.00 54. | | | C |
| | ATOM | 680 | CA | HIS . | A 4 | 5 | | 40.970 | 7.043 | 24.813 | 1.00 54. | | | c |
| 20 | ATOM | 682 | CB | HIS . | A 4 | 5. | | 40.782 | 6.831 | 23.332 | 1.00 50. | | | |
| | ATOM | 685 | CG | HIS . | A 4 | 5 | | 39.905 | 7.860 | 22.704 | 1.00 47. | | | C |
| | ATOM | 686 | | HIS. | | 5 | | 38.634 | 8.126 | 23.167 | 1.00 46. | | | N |
| | MOTA | 688 | | HIS | | 5 | | 38.094 | 9.082 | 22.429 | 1.00 49. | | | С |
| • | ATOM | 690 | | HIS | | 5 | | 38.965 | 9.443 | 21.501 | 1.00 40. | | | N |
| 25 | ATOM | 692 | | HIS | | 5 | | 40.108 | 8.692 | 21.654 | 1.00 46. | 25 | | C |
| 23 | ATOM | 694 | c | HIS | | 5 | | 39.645 | 7.185 | 25.525° | 1.00 61. | 01 | | С |
| • | ATOM | 695 | Ö | HIS | | 5 | | 38.869 | 6.236 | 25.629 | 1.00 68. | 54 | | 0 |
| | | 696 | N | PRO | | 6 | | 39.368 | 8.398 | 25.976 | 1.00 66. | 55 | | N |
| | ATOM | | CA | PRO | | 6 | | 38.316 | 8.630 | 26.973 | 1.00 67. | 17 | | С |
| 20 | ATOM | 697 | CB | PRO | | 6 | | 37.953 | 10.103 | 26.772 | 1.00 67. | | | С |
| 30 | MOTA | 699 | | | | 16 | | 39.078 | 10.729 | 25.902 | 1.00 64. | | | С |
| | MOTA | 702 | CG | PRO | | 6 | | 39.993 | 9.648 | 25.496 | 1.00 65. | | | С |
| | MOTA | 705 | CD | PRO | | | | 37.104 | 7.770 | 26.736 | 1.00 65. | | | С |
| • | MOTA | 708 | С | PRO | | 16 | | 36.433 | 7.311 | 27.650 | 1.00 68. | | | 0 |
| | MOTA | 709 | 0 | PRO | | 16 | • | | 7.530 | 25.479 | 1.00 62 | | | N |
| 35 | MOTA | 710 | N | | | 17 | | 36.823 | 6.833 | 25.156 | 1.00 60 | | ٠. | С |
| | MOTA | 712 | CA | PHE | | 17 | | 35.613 | | 23.806 | 1.00 58 | | | C |
| | MOTA | 714 | CB | PHE | | 17 | | 35.137 | 7.330 | 23.780 | 1.00 57 | | | c |
| | MOTA | 717 | CG | PHE | | 47 | | 34.910 | 8.805 | | 1.00 54 | | | Č |
| | ATOM | . 718 | | PHE | | 47 | | 34.809 | 9.490 | 22.583 | 1.00 50 | | | c |
| 40 | ATOM | 720 | | PHE | | 47 | | 34.602 | 10.831 | 22.559 | | | | c |
| | MOTA | 722 | CZ | PHE | | 47 | | 34.486 | 11.529 | 23.739 | 1.00 57 | | | Ċ |
| | ATOM | 724 | CE2 | PHE 2 | | 47 | | 34.583 | 10.865 | 24.944 | 1.00 60 | | | C |
| | MOTA | 726 | CD2 | PHE | Α | 47 | | 34.792 | 9.507 | 24.965 | 1.00 59 | | | c |
| | MOTA | 728 | С | PHE | Α | 47 | | 35.728 | 5.340 | 25.155 | 1.00 58 | | - | |
| 45 | MOTA | 729 | 0 | PHE | Α | 47 | | 34.806 | 4.684 | 24.721 | 1.00 61 | | | 0 |
| •- | ATOM | 730 | N | LEU | Α | 48 | | 36.829 | 4.774 | 25.625 | 1.00 58 | | | N |
| | ATOM | 732 | CA | LEU | Α. | 48 | | 36.896 | 3.322 | 25.635 | | | | C |
| | ATOM | 734 | СВ | LEU | | 48 | | 38.084 | 2.812 | 24.786 | | | | C. |
| | ATOM | 737 | CG | LEU | | 48 | | 38.037 | 3.121 | 23.271 | | .91 | | C |
| 50 | ATOM | 739 | | 1 LEU | | 48 | | 39.439 | 3.297 | 22.652 | 1.00 56 | .82 | | С |
| 50 | | 743 | | 2 LEU | | 48 | | 37.235 | 2.074 | 22.456 | | .09 | | С |
| | MOTA | | | LEU | | 48 | | 36.928 | 2.709 | 27.037 | | | | С |
| | ATOM | 747 | | LEU | | 48 | | 37.767 | 3.065 | 27.846 | | | | 0 |
| | MOTA | 748 | | | | | | 35.984 | | 27.305 | | | | N |
| | MOTA | 749 | | HIS | | 49 40 | | | | | | | | С |
| 55 | MOTA | 751 | CA | HIS | | 49 | | 36.036. | | 28.642 | | | | Ċ |
| • | MOTA | 753 | | | | 49 | | 34.791 | | | | | | Ċ |
| | MOTA | 756 | | | | 49 | | 33.560 | 0.785 | | | | | N |
| | MOTA | 757 | | 1 HIS | | 49 | | 33.631 | 2.037 | | | | | C |
| | ATOM | 759 | | 1 HIS | | 49 | | 32.415 | 2.503 | | | | | |
| 60 | ATOM | 761 | . NE | 2 HIS | | 49 | | 31.550 | 1.587 | | | | | N |
| | ATOM | 763 | | 2 HIS | Α | 49 | | 32.241 | 0.494 | 28.908 | 1.00 79 | .17 | | С |
| | | | | | | | | | | | | | | |

| 5 | ATOM | 765 | С | HIS A | 49 | 37. | 173 | -0.070 | 28.366 | 1.00 | 60.95 | | | C. |
|------|-------|-----|-----|-------|------|------|-------|--------|--------|------|-------|----|---|-----|
| , | ATOM | 766 | | HIS A | 49 | | 563 | -0.684 | 29.362 | 1.00 | 60.23 | | | 0 |
| | ATOM | 767 | | ARG A | 50 | | 669 | -0.304 | 27.149 | 1.00 | 58.11 | | | N |
| | | 769 | | ARG A | 50 | | 768 | -1.253 | 26.923 | 1.00 | 55.40 | | | С |
| | ATOM | | | ARG A | 50 | | 247 | -2.671 | 26.985 | | 55.21 | | | С |
| .4.0 | ATOM | 771 | CB | | | • | 757 | -2.807 | 26.821 | | 54.36 | | | C |
| 10 | MOTA | 774 | CG | ARG A | 50 | | | | 27.167 | | 48.77 | • | | Č |
| | MOTA | 777 | | ARG A | 50 | | .239 | -4.211 | | | 52.02 | | | N |
| | MOTA | 780 | NE | ARG A | 50 | | .083 | -4.540 | 26.350 | | | | | C |
| | MOTA | 782 | CZ | ARG A | 50 | | .594 | -5.760 | 26.210 | | 49.86 | | | |
| | ATOM | 783 | NH1 | ARG A | 50, | | .170 | -6.765 | 26.847 | | 49.97 | | | N |
| 15 | ATOM | 786 | NH2 | ARG A | 50. | . 33 | .529 | -5.971 | 25.440 | | 44.75 | | | N |
| | ATOM | 789 | С | ARG A | 50 | 39 | . 577 | -1.078 | 25.631 | | 56.08 | | | С |
| • | ATOM | 790 | 0 | ARG A | 50 | 39 | .388 | -0.103 | 24.861 | | 55.23 | | | 0 |
| | ATOM | 791 | N | TYR A | 51 | 40 | .506 | -2.013 | 25.413 | | 56.91 | | | N |
| | ATOM | 793 | CA | TYR A | 51 | | .319 | -2.010 | 24.195 | 1.00 | 57.53 | | | С |
| 20 | ATOM | 795 | CB | TYR A | 51 | | .153 | -0.735 | 24.085 | 1.00 | 58.76 | | | С |
| .20 | MOTA | 798 | CG | TYR A | 51 | | .220 | -0.483 | 25.148 | 1.00 | 65.10 | | | С |
| | | 799 | | TYR A | 51 | | .487 | -1.041 | 25.057 | | 70.53 | | | C |
| | MOTA | | | | 51 | | .460 | -0.792 | 26.036 | | 68.47 | | | С |
| | MOTA | 801 | | TYR A | | | .171 | 0.023 | 27.101 | | 64.05 | | | C |
| | ATOM | 803 | CZ | TYR A | 51 | | | | 28.077 | | 56.09 | | | ō |
| 25 | MOTA | 804 | OH | TYR A | 51 | | .091 | 0.286 | | | 65.65 | | | č |
| | MOTA | 806 | | TYR A | 51 | | .947 | 0.573 | 27.198 | | | | | c |
| | MOTA | 808 | | TYR A | 51 | | .971 | 0.328 | 26.222 | | 64.80 | | | C |
| | MOTA | 810 | С | TYR A | 51 | | .211 | -3.222 | 24.026 | | 56.08 | | | |
| | ATOM | 811 | 0 | TYR A | 51 | | .650 | -3.810 | 24.983 | | 63.38 | ٠. | | 0 |
| 30 | ATOM | 812 | N | TYR A | 52 | | .456 | -3.600 | 22.783 | | 56.18 | | | N |
| • | MOTA | 814 | CA | TYR A | 52 | 43 | .369 | -4.698 | 22.440 | | 54.65 | | | C |
| | ATOM | 816 | CB | TYR A | 52 | 43 | .609 | -4.634 | 20.954 | | 52.23 | | - | С |
| | ATOM | 819 | CG | TYR A | 52 | | .309 | -5.802 | 20.342 | | 49.44 | | - | C |
| | MOTA | 820 | CD1 | TYR A | 52 | 44 | .364 | -7.038 | 20.958 | 1.00 | 49.18 | | | Ċ |
| 35 | ATOM | 822 | | TYR A | 52 | | .014 | -8.084 | 20.352 | 1.00 | 44.95 | | | С |
| 33 | ATOM | 824 | CZ | TYR A | | | .598 | -7.880 | 19.123 | 1.00 | 40.40 | | | С |
| | ATOM | 825 | | TYR A | | | .257 | -8.880 | 18.453 | 1.00 | 43.51 | | | 0 |
| | MOTA | 827 | | TYR A | | | .543 | -6.683 | 18.523 | | 36.90 | | | С |
| | | 829 | | TYR A | | | .906 | -5.663 | 19.117 | | 44.53 | | | C |
| 40 | MOTA | 831 | C | TYR A | | | .716 | -4.512 | 23.090 | | 56.76 | | | С |
| 40 | MOTA | | | TYR A | | | .267 | -3.421 | 23.042 | | 61.43 | | | 0 |
| | MOTA | 832 | 0 | | | | .269 | -5.562 | 23.694 | | 58.49 | • | • | N |
| | MOTA | 833 | N | GLN A | | | .570 | -5.444 | 24.371 | | 50.39 | | | C |
| • | ATOM | 835 | CA | GLN A | | | | | | | 52.39 | | | Č |
| · | MOTA | 837 | СВ | GLN A | | | . 443 | -5.654 | | | 57.22 | | | Č |
| 45 | MOTA | 840 | CG | GLN A | | | .728 | -4.466 | 26.574 | | | | | Č |
| | ATOM | 843 | CD | GLN A | | | .807 | -4.475 | 28.089 | | 59.21 | | | |
| | ATOM | 844 | | GLN A | | | .778 | -4.523 | | | 68.21 | • | | 0 |
| | ATOM- | 845 | NE2 | GLN A | 53 | | .019 | -4.413 | 28.627 | | 60.90 | | | И |
| • | MOTA | 848 | С | GLN A | 53 | 47 | .498 | -6.427 | 23.723 | | 48.79 | | | C |
| 50 | MOTA | 849 | 0 | GLN A | 53 | 47 | .660 | -7.571 | 24.144 | 1.00 | 48.67 | | | 0 |
| | ATOM | 850 | N | ARG A | | 48 | 1.115 | -5.964 | 22.659 | | 44.44 | | | N |
| | ATOM | 852 | CA | ARG A | | 48 | 994 | -6.809 | 21.908 | 1.00 | 42.47 | | | C |
| | MOTA | 854 | СВ | ARG A | | | 669 | -5.949 | 20.864 | 1.00 | 42.10 | | | С |
| | ATOM | 857 | CG | ARG A | | | 3.733 | -5.430 | 19.740 | | 35.73 | | | С |
| 55 | | 860 | CD | ARG A | | | .465 | -4.449 | 18.787 | | 38.01 | | | С |
| در | MOTA | | | ARG A | | | 506 | -3.127 | 19.393 | | 46.13 | | | N |
| | MOTA | 863 | NE | | | | | -2.072 | 18.861 | | 54.49 | | | . C |
| | ATOM | 865 | CZ | ARG A | | | | | | | 63.14 | | | N |
| | MOTA | 866 | | ARG A | | | 0.646 | -2.176 | 17.682 | | 58.58 | | | N- |
| | MOTA | 869 | | ARG A | | | 0.052 | -0.903 | | | | | | C |
| 60 | MOTA | 872 | С | ARG A | | | 0.023 | ~7.562 | 22.802 | | 46.11 | | | |
| | MOTA | 873 | 0 | ARG A | 4 54 | 50 | 0.297 | -8.750 | 22.623 | 1.00 | 50.14 | | | 0 |
| | • | | | | | | | | | | | | | |

| _ | 7 m014 | 074 1 | N C | SLN A | 55 | | 50.583 | -6.887 | 23.777 | 1.00 4 | | | | N |
|------------|--------|------------|----------|----------------|-----|---|------------------|-----------|----------|--------|-------|---|----|--------|
| 5 | MOTA | - | | GLN A | | | 51.570 | -7.530 | 24.638 | 1.00 5 | | | | С |
| | ATOM | | | SLN A | | • | 52.120 | -6.504 | 25.638 | 1.00 5 | 6.89 | | | С |
| | MOTA | | | GLN A | | | 51.331 | -5.158 | 25.639 | 1.00 6 | 3.64 | | | C, |
| | ATOM | | | GLN A | | | 50.389 | -4.991 | 26.815 | 1.00 6 | 9.23 | | | С |
| | MOTA | | | GLN A | | | 49.575 | -4.052 | 26.852 | 1.00 6 | | | | 0 |
| 10 | ATOM | | OPT (| GLN A | 55 | | 50.502 | -5.892 | 27.790 | 1.00 7 | 5.17 | | | N |
| | MOTA | | | | | | 51.054 | -8.780 | 25.379 | 1.00 5 | 6.17 | | | С |
| | ATOM | | | GLN A | _ | | 51.849 | -9.509 | 25.952 | 1.00 5 | 5.62 | | | 0 |
| | MOTA | | • | GLN A | | | 49.750 | -9.047 | 25.388 | 1.00 5 | 5.53 | | | N |
| | | | | LEU A | | | | -10.216 | 26.133 | 1.00 5 | 6.08 | | | С |
| 15 | ATOM | - | | LEU A | | | 48.009 | -9.835 | 26.904 | 1.00 5 | | | - | C |
| • | MOTA | | | LEU A | | | 48.155 | -8.608 | 27.785 | 1.00 6 | 51.56 | | | С |
| • | ·ATOM | | | LEU A LEU A | _ | - | 46.968 | -8.502 | 28.711 | 1.00 6 | 52.62 | ~ | | C |
| | MOTA | | | | | | 49.453 | -8.699 | 28.580 | 1.00 | | | | С |
| | MOTA | - | | LEU A | | | | -11.462 | 25.352 | 1.00 5 | | | | С |
| 20 | MOTA | - | - | LEU A | | | 40.074 | -12.472 | 25.953 | 1.00 5 | | | | 0 |
| | ATOM | | | LEU A | | | 18 965 | -11.396 | 24.029 | 1.00 5 | | | | N . |
| | MOTA | - | | SER F | | | 40.503 48.533 | -12.496 | 23.198 | 1.00 ! | | | | С |
| | MOTA | 912 | | SER A | | | | -12.011 | 22.060 | 1.00 | 50.76 | | | С |
| | MOTA | 914 | | SER F | | | 47.074 | -13.069 | 21.154 | 1.00 | 51.82 | | | Ο. |
| 25 | ATOM | 917 | OG | SER A | | | | -13.087 | 22.633 | 1.00 | | | | С |
| | MOTA | 919 | С | SER A | | | | -12.386 | 22.229 | 1.00 | | | | 0 |
| | ATOM | 920 | 0 | SER A | | | | -14.384 | 22.582 | 1.00 | 51.36 | | | N |
| | MOTA | 921 | N | SER A | | | 51 036 | -14.980 | 22.152 | 1.00 | | • | | С |
| | ATOM | 923 | CA | SER A | | | | -16.234 | 22:948 | 1.00 | | | | C. |
| 30 | ATOM | 925 | CB | SER A | | | 50 240 | -17.142 | 22.588 | 1.00 | | | ٠. | 0 |
| | MOTA | 928 | OG | SER A | | | 50.240 | -15.342 | 20.717 | 1.00 | | | | C, |
| | MOTA | 930 | С | SER A | | | 51 810 | -15.932 | 20.154 | 1.00 | | | | 0 |
| | MOTA | 931 | 0 | SER A | | | | -15.005 | 20.122 | 1.00 | | | | N |
| | ATOM | 932 | N | THR | | | | -15.299 | | 1.00 | | | | С |
| 35 | MOTA | 934 | CA | THR | | | 49.331 | -15.986 | | | 43.26 | | | С |
| | MOTA | 936 | CB | THR . | | | 47 220 | -15.363 | | 1.00 | 40.46 | | | 0 |
| | MOTA | 938 | | THR | | | 48 237 | -17.366 | | 1.00 | 43.84 | | • | С |
| | MOTA | 940 | CGZ | THR | | | 49.674 | -13.990 | | 1.00 | 48.17 | | | С |
| 40 | MOTA | 944 | 0 | THR | | | | -13.981 | | | 49.26 | | | 0 |
| 40 | MOTA | 945 | | TYR | | | 50.023 | -12.884 | | 1.00 | 44.42 | | | N |
| ÷ | ATOM | 946 | N | TYR | | | | -11.625 | | 1.00 | 45.38 | | | С |
| | MOTA | 948 | CA CB | TYR | | | | -10.499 | | 1.00 | 46.42 | | | C |
| | ATOM | 950 | CG | TYR | | | 50.852 | | | | 46.69 | | | C. |
| 45 | MOTA | 953 954 | | TYR | | | 49.94 | | | | 47.22 | | | C C |
| 45 | ATOM | 954 | | TYR | | | 50.29 | | | | 47.17 | | | C |
| | ATOM | 958 | CZ | TYR | | | 51.54 | | | | 44.65 | | | C |
| | MOTA | 959 | OH | TYR | | | 51.89 | | 16.408 | 1.00 | 49.47 | | | 0 |
| - | MOTA | - | | TYR | | - | 52.44 | | _ | 1.00 | 41.96 | | | C |
| 50 | ATOM | 961 | | TYR | | | 52.10 | | | | 45.55 | | | C |
| 50 | ATOM | 963 | C | TYR | | | 51.32 | 5 -11.709 | | 1.00 | 47.40 | | | С |
| | ATOM | 965 | Ö | TYR | | | 52.26 | 2 -12.460 | 17.080 | 1.00 | 51.21 | | | 0 |
| | ATOM | 966 | N. | ARG | | | 51.24 | 9 -10.942 | 15.804 | 1.00 | 48.35 | | | N. |
| | MOTA | 967 | | ARG | | | 52.38 | 8 -10.78 | | | 41.23 | | | С |
| | MOTA | 969 | CA CB | ARG | | | 52.39 | 2 -11.782 | 2 13.795 | 1.00 | 44.25 | | | C |
| 55 | MOTA | 971 | * | ARG | | | 52.54 | 8 -13.20 | 5 14.213 | 3 1.00 | 45.20 | | | С |
| | ATOM | 974 | CG | ARG | | | 52.37 | 5 -14.11 | 8 13.033 | | 46.69 | | | С |
| | MOTA | 977 | CD NE | ARG | | | 53.34 | 3 -15.39 | | | 51.89 | | | N |
| | MOTA | 980 | CZ | ARG | | | 52.89 | 3 -16.54 | | 6 1.00 | 51.83 | | | С |
| (0 | MOTA | 982 | | ARG 1 ARG | | | 51 . 87 | 2 -16.57 | 5 12.24 | | 59.34 | | | N |
| 60 | MOTA | 983 | | | | | 53 44 | 8 -17.66 | 8 13.48 | | 50.67 | | | · N |
| | MOTA | 986 | MH. | 2 ARG | A O | _ | 33.47 | | | | | | | |

| 5 | MOTA | 989 | С | ARG | Α | 61 | | 52.287 | -9.433 | 14.302 | 1.00 41 | | | | С |
|----|------|------|-----|-----|-----|-----|----|--------|--------|--------|---------|------|---|---|------|
| | MOTA | 990 | 0 . | ARG | A | 61 | | 51.278 | -9.127 | 13.687 | 1.00 38 | | | | 0 |
| | MOTA | 991 | N | ASP | Α | 62 | | 53.374 | -8.681 | 14.477 | 1.00 45 | | | | N |
| | ATOM | 993 | CA | ASP | A | 62 | | 53.654 | -7.322 | 13.990 | 1.00 43 | | | | C |
| | ATOM | 995 | CB | ASP | Ä | 62 | | 54.947 | -6.899 | 14.658 | 1.00 46 | | | | С |
| 10 | ATOM | 998 | CG | ASP | Α | 62 | | 55.158 | -5.405 | 14.673 | 1.00 50 | | | | С |
| | ATOM | 999 | OD1 | ASP | Α | 62 | | 54.562 | -4.701 | 13.833 | 1.00 47 | .18 | | | 0 |
| | ATOM | 1000 | OD2 | ASP | A | 62 | | 55.940 | -4.872 | 15.520 | 1.00 56 | .56 | | | 0 |
| | MOTA | 1001 | С | ASP | Α | 62 | | 53.950 | -7.230 | 12.530 | 1.00 38 | .57 | | | С |
| | ATOM | 1002 | 0 | ASP | Α | 62 | | 54.868 | -7.840 | 12.078 | 1.00 34 | .49 | | | 0 |
| 15 | ATOM | 1003 | N | LEU | Α | 63 | | 53.204 | -6.429 | 11.784 | 1.00 42 | | | | N |
| | ATOM | 1005 | CA | LEU | A | 63 | | 53.464 | -6.332 | 10.355 | 1.00 41 | . 63 | | | С |
| | MOTA | 1007 | CB | LEU | Α | 63 | | 52.131 | -6.216 | 9.586 | 1.00 39 | | | | C |
| | ATOM | 1010 | CG | LEU | Α | 63 | | 51.262 | -7.490 | 9.430 | 1.00 39 | | | | С |
| • | ATOM | 1012 | CD1 | LEU | Α | 63 | | 49.768 | -7.233 | 9.242 | 1.00 38 | | | | С |
| 20 | ATOM | 1016 | CD2 | LEU | Α . | 63 | | 51.755 | -8.283 | 8.272 | 1.00 35 | .93 | | | C |
| | ATOM | 1020 | С | LEU | Α | 63 | | 54.414 | -5.180 | 10.024 | 1.00 45 | 5.54 | | | С |
| | ATOM | 1021 | 0 | LEU | A | 63 | | 54.659 | -4.921 | 8.853 | 1.00 45 | | | | 0 |
| | ATOM | 1022 | N | ARG | Α | 64 | | 54.933 | -4.467 | 11.034 | 1.00 47 | | | | N |
| | ATOM | 1024 | CA | ARG | Α | 64 | | 55.873 | -3.385 | 10.779 | 1.00 45 | .84 | | | С |
| 25 | ATOM | 1026 | CB | ARG | | 64 | | 57.261 | -3.976 | 10.447 | 1.00 46 | 5.95 | | | С |
| | MOTA | 1029 | CG | ARG | Α | 64 | | 57.974 | -4.717 | 11.615 | 1.00 48 | 3.68 | | | С |
| | MOTA | 1032 | CD | ARG | Α | 64 | | 58.685 | -6.010 | 11.233 | 1.00 49 | 84 | | | C |
| | MOTA | 1035 | NE | ARG | | 64 | | 59.846 | -5.810 | 10.371 | 1.00 52 | | | | N |
| | MOTA | 1037 | ·CZ | ARG | A | 64 | • | 60.138 | -6.547 | 9.301 | 1.00 58 | 3.00 | | | С |
| 30 | ATOM | 1038 | NH1 | ARG | Α | 64 | | 59.360 | -7.557 | 8.918 | 1.00 57 | | | | N |
| | ATOM | 1041 | NH2 | ARG | Α | 64 | | 61.220 | -6.268 | 8.594 | 1.00 59 | | | | N |
| | ATOM | 1044 | С | ARG | Α. | 64 | | 55.451 | -2.492 | 9.608 | 1.00 51 | 1.03 | | | С |
| | MOTA | 1045 | 0 | ARG | A | 64 | | 56.259 | -2.219 | 8.721 | 1.00 53 | | | | 0 |
| | ATOM | 1046 | N | LYS | A | 65 | | 54.198 | -2.035 | 9.584 | 1.00 53 | 3.47 | | • | N |
| 35 | ATOM | 1048 | CA | LYS | Α | 65 | | 53.686 | -1.175 | 8.489 | 1.00 51 | L.33 | | | С |
| • | ATOM | 1050 | CB | LYS | A | 65 | | 53.329 | -2.050 | 7.229 | 1.00 48 | 3.60 | | | С |
| | ATOM | 1053 | CG | LYS | A | 65 | | 52.131 | -1.667 | 6.219 | 1.00 48 | 3.91 | | | С |
| | MOTA | 1056 | CD | LYS | A | 65 | | 51.911 | -2.702 | 4.881 | 1.00 50 | 0.16 | | | , C |
| | MOTA | 1059 | CE | LYS | Α | 65 | | 50.792 | -4.019 | 4.900 | 1.00 4 | | | | С |
| 40 | MOTA | 1062 | NZ | LYS | A | 65 | | 51.193 | -5.488 | 4.701 | 1.00 1 | | | | N |
| | MOTA | 1066 | С | LYS | A | 65 | | 52.519 | -0.436 | 9.136 | 1.00 5 | | | | С |
| | MOTA | 1067 | 0 | LYS | Α | 65 | | 51.705 | -1.075 | 9.781 | 1.00 5 | | | | 0 |
| | MOTA | 1068 | N. | GLY | A | 66 | | 52.450 | 0.890 | 9.005 | 1.00 4 | | | | N |
| | ATOM | 1070 | CA | GLY | Α | 66 | | 51.359 | 1.678 | 9.588 | 1.00 4 | | | | C |
| 45 | MOTA | 1073 | C | GLY | Α | 66 | - | 50.196 | 1.971 | 8.628 | 1.00 4 | | | | C |
| • | MOTA | 1074 | 0 | GLY | Α | 66 | | 50.277 | 1.787 | 7.418 | 1.00 4 | | | | 0 |
| | MOTA | 1075 | N | VAL | Α | 67 | • | 49.095 | 2.470 | 9.152 | 1.00 3 | | | | N |
| | MOTA | 1077 | CA | VAL | A | 67 | | 48.000 | 2.820 | 8.264 | 1.00 3 | | | | С |
| | MOTA | 1079 | CB | VAL | A | 67 | | 47.307 | 1.531 | 7.793 | 1.00 3 | | | | · C |
| 50 | MOTA | 1081 | CG1 | VAL | Α | 67 | | 46.878 | 0.663 | 8.984 | 1.00 3 | | • | | C |
| | MOTA | 1085 | CG2 | VAL | Α | 67 | | 46.129 | 1.806 | 6.999 | 1.00 3 | 3.52 | | | C |
| | ATOM | 1089 | C | VAL | Α | 67 | | 47.021 | 3.841 | 8.882 | 1.00 4 | 0.42 | | | С |
| | MOTA | 1090 | 0 | VAL | Α | 67 | ٠. | 46.885 | 3.969 | | 1.00 4 | 0.64 | | | 0 |
| | ATOM | 1091 | N· | | | 68 | | 46.352 | 4.546 | 7.971 | 1.00 4 | 5.72 | | | · N. |
| 55 | ATOM | 1093 | CA | TYR | | 68 | | 45.436 | 5.668 | 8.208 | 1.00 4 | 6.34 | | | C. |
| | ATOM | 1095 | CB | TYR | Α | 68. | | 46.052 | 6.874 | 7.536 | 1.00 5 | 1.19 | | | , C |
| | ATOM | 1098 | CG | TYR | Α | 68 | | 45.306 | 8.202 | 7.533 | 1.00 6 | 1.31 | | | С |
| | ATOM | 1099 | CD1 | TYR | | 68 | | 44.911 | 8.826 | 8.726 | 1.00 6 | 2.21 | | | C |
| | ATOM | 1101 | | TYR | | 68 | | 44.266 | 10.043 | 8.702 | 1.00 6 | 1.39 | | | С |
| 60 | ATOM | 1103 | CZ | TYP | | 68 | | 44.008 | 10.665 | 7.491 | 1.00 6 | | | | С |
| | ATOM | 1104 | OH | TYF | | 68 | | 43.361 | 11.886 | 7.472 | 1.00 6 | 6.32 | • | | 0 |
| | | | | | | | | | | | | | | | |

| 5 | ATOM | 1106 | CE2 | TYR 2 | Α. | 68 | | 44.390 | 10.080 | 6.298 | 1.00 58.19 | | | С |
|-----|--------|------|-----|-------|----|-----|---|--------|--------|--------|------------|-----|-------|-----|
| , | ATOM | 1108 | | TYR | | 68 | | 45.039 | 8.864 | 6.321 | 1.00 61.27 | • | | С |
| | ATOM | 1110 | | TYR : | | 68 | | 44.152 | 5.440 | 7.505 | 1.00 41.55 | | | C |
| | ATOM | 1111 | | TYR | | 68 | | 44.130 | 5.185 | 6.335 | 1.00 42.23 | | | 0 |
| | MOTA | 1112 | | VAL | | 69 | | 43.045 | 5.557 | 8.195 | 1.00 45.73 | | | N |
| 10. | | 1114 | | VAL . | | 69 | | 41.791 | 5.348 | 7.519 | 1.00 43.18 | | • | С |
| 10 | MOTA | 1114 | | VAL . | | 69 | | 41.256 | 3.958 | 7.920 | 1.00 46.99 | | | С |
| | MOTA | 1118 | | VAL . | | 69 | | 39.856 | 3.712 | 7.399 | 1.00 46.87 | | | C. |
| | ATOM | 1112 | | VAL . | | 69 | • | 42.216 | 2.897 | 7.399 | 1.00 39.84 | | | С |
| | ATOM | | | VAL | | 69 | | 40.831 | 6.478 | 7.832 | 1.00 37.88 | | | С |
| 1.6 | ATOM | 1126 | C | | | 69 | | 40.436 | 6.622 | 8.962 | 1.00 45.27 | | | 0 |
| 15 | ATOM | 1127 | 0 | VAL . | | 70 | | 40.497 | 7.286 | 6.823 | 1.00 34.02 | | | N |
| | ATOM | 1128 | N | PRO . | | 70 | | 39.507 | 8.345 | 6.917 | 1.00 29.99 | | | С |
| | ATOM | 1129 | CA | PRO | | 70 | - | 40.071 | 9.345 | 5.934 | 1.00 26.73 | | | C |
| | ATOM . | 1131 | 7,1 | | | | | 40.414 | 8.518 | 4.800 | 1.00 25.36 | | | C |
| ó۵ | MOTA | 1134 | CG | PRO | | 70 | | | 7.267 | 5.456 | 1.00 34.53 | | | č |
| 20 | MOTA | 1137 | CD | PRO | | 70 | | 41.047 | | 6.383 | 1.00 35.42 | | | Č |
| | MOTA | 1140 | С | PRO | | 70 | | 38.118 | 7.941 | | 1.00 35.66 | | | ŏ |
| | ATOM | 1141 | 0 | PRO | | 70 | • | 37.992 | 7.309 | 5.318 | 1.00 33.00 | | | N |
| | MOTA | 1142 | N | TYR | | 71 | | 37.067 | 8.315 | 7.102 | 1.00 47.40 | | | C |
| | ATOM | 1144 | CA | TYR | | 71 | | 35.699 | 8.076 | | 1.00 47.40 | | | C |
| 25 | MOTA | 1146 | CB | TYR | | .71 | | 34.943 | 7.305 | 7.684 | | | | C |
| | MOTA | 1149 | CG | TYR | | 71 | | 35.651 | 6.025 | 8.159 | 1.00 49.56 | | | c |
| | ATOM | 1150 | CD1 | | | 71 | | 35.181 | 4.750 | 7.818 | 1.00 49.21 | | | C |
| | MOTA | 1152 | CE1 | TYR | | 71 | | 35.822 | 3.609 | 8.258 | 1.00 46.98 | | | ¢ |
| | MOTA | 1154 | CZ | TYR | | 71 | • | 36.924 | 3.741 | 9.045 | 1.00 44.80 | | · | |
| 30 | MOTA | 1155 | OH | TYR | | 71 | | 37.601 | 2.666 | 9.526 | 1.00 46.04 | | | 0 |
| | MOTA | 1157 | | TYR | | 71 | | 37.387 | 4.972 | 9.389 | 1.00 50.64 | | | С |
| | MOTA | 1159 | | TYR | | 71 | | 36.756 | 6.097 | 8.949 | 1.00 50.58 | | | C |
| ٠. | MOTA | 1161 | С | TYR | | 71 | | 34.974 | 9.409 | 6.253 | 1.00 51.01 | | | С |
| | MOTA | 1162 | 0 | TYR | | 71 | | 35.607 | 10.448 | 6.041 | 1.00 56.69 | | | 0 |
| 35 | MOTA | 1163 | N | THR | Α | 72 | | 33.653 | 9.373 | 6.144 | 1.00 54.00 | | | N |
| | MOTA · | 1165 | CA | THR | | 72 | | 32.842 | 10.586 | 5.982 | 1.00 48.48 | | | C |
| | ATOM | 1167 | CB | THR | | 72 | | 31.462 | 10.140 | 5.541 | 1.00 42.99 | | | С |
| | MOTA | 1169 | OG1 | | | 72 | | 31.614 | 9.334 | 4.387 | 1.00 44.3 | | | 0 |
| | MOTA | 1171 | CG2 | THR | | 72 | | 30.620 | 11.232 | 4.935 | 1.00 46.38 | | | C |
| 40 | ATOM | 1175 | С | THR | Α | 72 | | 32.834 | 11.426 | 7.291 | 1.00 50.7 | | • | C |
| | ATOM | 1176 | 0 | THR | Α | 72 | • | 32.793 | 12.633 | 7.256 | 1.00 49.8 | | • | 0 |
| | MOTA | 1177 | N | GLN | Α | 73 | | 32.873 | 10.790 | 8.446 | 1.00 57.0 | | | N |
| | MOTA | 1179 | CA | GLN | Α | 73 | | 33.020 | 11.507 | 9.717 | 1.00 61.3 | | | С |
| | MOTA | 1181 | CB | GLN | Α | 73 | | 31.704 | 11.705 | 10.489 | 1.00 61.8 | | | С |
| 45 | MOTA | 1184 | CG | GLN | Α | 73 | | 30.932 | 13.008 | 10.237 | 1.00 69.0 | | | С |
| | MOTA | 1187 | CD | GLN | A | 73 | | 31.616 | 14.250 | 10.830 | 1.00 73.5 | | | С |
| | MOTA | 1188 | OE1 | GLŅ | A | 73 | | 31.469 | 14.561 | 12.028 | 1.00 73.4 | | | 0 |
| | MOTA | 1189 | NE2 | GLN | Α | 73 | | 32.369 | 14.960 | 9.987 | 1.00 74.6 | | | N |
| | ATOM | 1192 | С | GLN | Α | 73 | | 33.930 | 10.654 | 10.576 | 1.00 61.5 | 3 | • | C |
| 50 | MOTA | 1193 | 0 | ĢLN | | 73 | | 33.592 | 9.520 | 10.910 | 1.00 63.2 | | | 0 |
| | ATOM | 1194 | N | GLY | | 74 | | 35.079 | 11.208 | 10.935 | 1.00 62.0 | 4 | | N |
| | MOTA | 1196 | CA | GLY | | 74 | | 36.019 | 10.538 | 11.816 | 1.00 60.6 | 6 | • | ç |
| | MOTA | 1199 | С | GLY | | 74 | • | 37.207 | 9.927 | 11.093 | 1.00 54.0 | 1 | • • • | |
| | MOTA | 1200 | Ó | GLY | | 74 | | 37:126 | 9.641 | 9.901 | 1.00 47.5 | 1 . | | · O |
| 55 | ATOM | 1201 | N | LYS | | 75 | | 38.310 | 9.754 | 11.822 | 1.00 51.5 | | | N |
| رر | ATOM | 1203 | | LYS | | 75 | • | 39.445 | 8.982 | 11.330 | 1.00 48.5 | | | С |
| ٠. | MOTA | 1205 | CB | LYS | | 75 | | 40.395 | 9.783 | 10.472 | 1.00 49.3 | | | C |
| | ATOM | 1203 | CG | LYS | | 75 | | 40.953 | 11.042 | 11.076 | 1.00 50.3 | | | С |
| | | 1211 | CD | LYS | | 75 | | 41.467 | 11.932 | 9.917 | 1.00 49.2 | | | C |
| 60 | MOTA | 1211 | CE | LYS | | | | 41.609 | 13.425 | 10.286 | 1.00 50.5 | | | C |
| 60 | MOTA | | NZ | LYS | | | | 43.031 | 13.815 | 10.654 | 1.00 42.6 | | | N |
| | MOTA | 1217 | NA | nto | ч | 13 | | 43.031 | 10.010 | 10.004 | 12.0 | • | | |

| 5 | ATOM | 1221 | С | LYS A | A | 75 | | 40.203 | 8.425 | 12.455 | | 45.88 | | ** | |
|----|------|-------|--------|------------|-----|----------|---|--------|---------|--------|------|---------|---|----|----|
| Τ. | MOTA | 1222 | 0 | LYS A | A | 75 | | 39.958 | 8.795 | 13.599 | | 46.47 | | | 0 |
| | ATOM | 1223 | N | TRP A | A | 76 | | 41.105 | 7.501 | 12.110 | | 46.31 | | | N |
| | ATOM | 1225 | CA | TRP A | A | 76 | | 42.052 | 6.881 | 13.058 | | 47.24 | | | C |
| | MOTA | 1227 | CB | TRP I | A | 76 | | 41.502 | 5.620 | 13.777 | | 41.96 | | | C |
| 10 | ATOM | 1230 | | TRP | | 76 | | 40.864 | 4.653 | 12.875 | | 40.56 | | | C |
| 10 | ATOM | 1231 | | TRP | | 76 | | 39.552 | 4.578 | 12.592 | | 42.47 | | | С |
| | ATOM | 1233 | | TRP | | 76 | | 39.304 | 3.557 | 11.706 | | 44.26 | | | N |
| - | MOTA | 1235 | | TRP . | | 76 | | 40.488 | 2.949 | 11.407 | | 40.38 | | | С |
| | ATOM | 1236 | | TRP | | 76 | | 41.494 | 3.615 | 12.132 | | 39.72 | | | С |
| 15 | ATOM | 1237 | | TRP | | 76 | | 42.814 | 3.176 | 11.996 | | 43.23 | • | | С |
| 13 | ATOM | 1239 | | TRP | | 76 | | 43.082 | 2.116 | 11.157 | 1.00 | 34.09 | | | C |
| | ATOM | 1241 | | TRP | | 76 | | 42.047 | 1.481 | 10.452 | | 40.84 | | | С |
| | ATOM | 1243 | | TRP | | 76 | | 40.749 | 1.887 | 10.567 | | 37.49 | | | С |
| | ATOM | 1245 | C. | TRP | | 76 | | 43.352 | 6.572 | 12.283 | 1.00 | 46.65 | | - | С |
| 20 | | 1246 | Ö | TRP | | 76 | | 43.376 | 6.593 | 11.058 | 1.00 | 44.54 | • | | 0 |
| 20 | MOTA | 1247 | N | GLU | | 77 | | 44.417 | 6.302 | 13.025 | 1.00 | 44.45 | | | N |
| | MOTA | 1249 | CA | GLU | | 77 | | 45.726 | 6.056 | 12.465 | 1.00 | 49.78 | | | С |
| | ATOM | 1251 | CB | GLU | | 77 | | 46.637 | 7.292 | 12.696 | 1.00 | 54,17 | | | С |
| | ATOM | | CG | GLU - | | 77 | | 45.798 | 8.559 | 12.966 | 1.00 | 63.47 | | | С |
| 25 | MOTA | 1254 | CD | GLU | | 77 | | 46.260 | 9.861 | 12.296 | | 65.72 | - | | С |
| 25 | MOTA | 1257 | | GLU | | 77 | | 47.499 | 10.099 | 12.217 | | 62.94 | | | 0 |
| | MOTA | 1258 | | GLU | | 77 | | 45.341 | 10.642 | 11.855 | | 57.77 | | | 0 |
| | ATOM | 1259 | C C | GLU | | 77 | | 46.145 | 4.851 | 13.268 | | 48.59 | | | С |
| | MOTA | 1260 | | GLU | | 77 | | 45.835 | 4.787 | 14.477 | | 46.46 | | | 0 |
| 20 | ATOM | 1261 | 0 | | | 78 | | 46.814 | 3.881 | 12.643 | | 44.59 | | | N |
| 30 | MOTA | 1262 | N | GLY | | 78 | | 47.148 | 2.670 | 13.387 | | 43.33 | | | C. |
| | MOTA | 1264 | CA | GLY GLY | | 78 | | 48.378 | 1.905 | 12.935 | | 45.34 | | | C |
| | MOTA | 1267 | C | | | 78 | | 49.054 | 2.322 | 11.945 | | 46.85 | | | 0 |
| | ATOM | 1268 | 0 | GLY | | 79 | | 48.635 | 0.805 | | | 40.38 | | | N |
| 25 | ATOM | 1269 | N | GLU | | 79 | | 49.702 | -0.144 | 13.391 | | 45.02 | | | С |
| 35 | ATOM | 1271 | CA | GLU | | 79 | | 50.631 | -0.248 | 14.675 | | 51.34 | | | Ç |
| | ATOM | 1273 | CB | GLU | | 79 | | 51.478 | 1.000 | 15.101 | | 55.46 | | | С |
| | ATOM | 1276 | CG | GLU | | 79 | | 52.047 | 0.912 | 16.565 | | 65.73 | | | С |
| | MOTA | 1279 | CD | GLU | | 79 | | 52.921 | 1.815 | 17.021 | | 64.66 | | | 0 |
| 40 | MOTA | 1280 | | GLU | | 79 | | 51.612 | -0.082 | 17.271 | | 54.33 | | | 0 |
| 40 | MOTA | 1281 | | GLU. | | | | 49.162 | -1.565 | 12.952 | | 44.43 | | | С |
| | MOTA | 1282 | C | GLU | | 79 | | 48.318 | -2.183 | 13.626 | | 39.67 | | | 0 |
| | MOTA | 1283 | 0 | GLU | | 79 | | 49.666 | -2.103 | 11.829 | | 45.33 | | | N |
| | MOTA | 1284 | N | LEU | | 80 80 | | 49.240 | -3.386 | 11.250 | | 42.70 | | | С |
| | ATOM | 1286 | CA | LEU | | | | 49.454 | -3.355 | 9.743 | | 39.42 | | | ·C |
| 45 | MOTA | 1288 | CB | LEU | | 80 | | | -2.502 | 9.024 | | 38.72 | | | С |
| | MOTA | 1291 | CG | LEU | | 80 | | 48.461 | -2.614 | 7.556 | | 0 41.48 | | | С |
| | MOTA | 1293 | | LEU | | 80 | | | | 9.427 | | 0 43.39 | • | | C |
| | MOTA | 1297 | | LEU | | 80 | | 47.097 | -2.967 | | | 0 42.16 | | | Ċ |
| | ATOM | 1301 | | LEU | | 80 | | 49.908 | -4.689 | | 1.0 | 0 39.15 | • | | ō |
| 50 | ATOM | 1302 | | | | 80 | | 51.133 | -4.789 | | | | | | N |
| | MOTA | 1,303 | N | GLY | | 81 | | 49.084 | ~5.715 | | | 0 38.15 | • | | C |
| | MOTA | 1305 | CA | GLY | | 81 | | 49.519 | -6.972 | | | 0 40.41 | | | c |
| | MOTA | 1308 | С | GLY | | | • | 48.517 | -8.073 | | | 0 41.89 | | | 0 |
| | MOTA | 1309 | 0 | GLY | | 81 | | 47.680 | -7.948 | | | 0 40.94 | | | |
| 55 | ATOM | 1310 | N | THR | | 82 | | 48.631 | -9.167 | | | 0 45.69 | | | N. |
| | ATOM | 1312 | | | | 82 | | 47.663 | -10.265 | 12.824 | | 0 41.72 | | | C |
| | ATOM | 1314 | CB | THR | | 82 | | 48.071 | -11.342 | 11.837 | | 0 41.41 | | | C |
| | MOTA | 1316 | | 1 THR | l A | 82 | | 49.268 | -12.009 | 12.302 | | 0 40.17 | | | 0 |
| | MOTA | 1318 | | | | | | 48.423 | -10.774 | 10.506 | | 0 39.10 | | | C |
| 60 | ATOM | 1322 | | THE | | | | | -10.947 | | | 0 42.06 | | | C |
| | ATOM | 1323 | | THE | R A | 82 | | 48.416 | -10.779 | 15.077 | 1.0 | 0 41.59 | | • | 0 |
| | | | | | | | | | | | | | | | |

| 5 | ATOM | 1324 | N | ASP | A | 83 | 46.532 -11.736 | 14.315 | 1.00 39.43 | N |
|-----|------|-------|-------|-----|----|------|----------------|--------|------------|------------|
| | ATOM | 1326 | CA | ASP | | 83 | 46.344 -12.449 | | 1.00 41.41 | Č |
| | ATOM | 1328 | CB | ASP | | 83 | 46.090 -11.482 | | 1.00 40.00 | č |
| | ATOM | 1331 | CG | ASP | | 83 | 46.263 -12.135 | | 1.00 44.18 | Č |
| | ATOM | 1332 | | ASP | | 83 | 46.475 -13.344 | | 1.00 45.61 | 0 |
| 10 | ATOM | 1333 | | ASP | | .83 | | | | |
| 10 | | | | | | | 46.225 -11.551 | | 1.00 52.07 | 0 |
| | ATOM | 1334 | C | ASP | | 83 | 45.163 -13.314 | | 1.00 44.90 | C |
| | ATOM | 1335 | 0 | ASP | | 83 | 44.544 -13.136 | | 1.00 51.63 | Ó |
| | ATOM | 1336 | N | LEU | | 84 | 44.847 -14.260 | • | 1.00 45.58 | 'n |
| 1.5 | ATOM | 1338€ | | LEU | | 84 | 43.699 -15.139 | | 1.00 44.62 | С |
| 15 | ATOM | 1340 | CB | LEU | | 84 | 43.951 -16.446 | | 1.00 41.76 | С |
| | MOTA | 1343 | CG | LEU | | 84 | 45.078 -17.361 | 16.133 | 1.00 41.81 | . C |
| | ATOM | 1345 | CD1 | LEU | Α. | 84 | 45.177 -18.491 | 17.103 | 1.00 46.46 | С |
| | ATOM | 1349 | CD2 | LEU | Α | 84 | 44.847 -17.978 | 14.767 | 1.00 42.92 | - C |
| • | MOTA | 1353 | С | LEU | Α | 84 | 42.374 -14.468 | 16.315 | 1.00 41.20 | С |
| 20 | ATOM | 1354 | 0 | LEU | A | 84 | 42.388 -13.643 | | 1.00 52.36 | 0 |
| | ATOM | 1355 | N | VAĹ | | 85 | 41.234 -14.803 | | 1.00 41.48 | N |
| | ATOM | 1357 | CA | VAL | Α | 85 | 39.973 -14.143 | | 1.00 37.87 | c |
| | ATOM | 1359 | CB | VAL | | 85 | 39.743 -12.994 | | 1.00 41.53 | Č |
| | ATOM | 1361 | | VAL | | 85 | 38.437 -12.345 | | 1.00 47.66 | č |
| 25 | ATOM | 1365 | | VAL | | 85 | 40.822 -11.985 | | 1.00 41.79 | C |
| | ATOM | 1369 | | VAL | | 85 | 38.680 -14.998 | | 1.00 39.48 | · c |
| | ATOM | 1370 | .0 | VAL | | 85 | 38.448 -15.737 | | 1.00 33.48 | |
| • | ATOM | 1371 | N | SER | | | 37.833 -14.882 | | | 0 |
| • | ATOM | 1373 | | SER | | 86 | | | 1.00 40.31 | N |
| 30 | | | | | | | 36.564 -15.608 | | 1.00 44.63 | |
| 50 | MOTA | 1375 | CB | SER | | 86 | 36.474 -16.510 | | 1.00 41.82 | · c |
| | ATOM | 1378 | OG | SER | | 86 | 37.738 -17.097 | | 1.00 55.30 | · O |
| | ATOM | | . C · | SER | | 86 | 35.365 -14.678 | | 1.00 45.48 | С |
| | ATOM | 1381 | 0. | SER | | 86 | 35.525 -13.486 | | 1.00 41.16 | O- |
| 25 | ATOM | 1382 | N | ILE | | 87 | 34.185 -15.266 | | 1.00 43.04 | N |
| 35 | ATOM | | CA | ILE | | 87 | 32.885 -14.643 | | 1.00 41.10 | C |
| | ATOM | 1386 | CB | ILE | | 87 | 32.215 -14.421 | 15.706 | 1.00 42.65 | С |
| | ATOM | 1388 | | ILE | | 87 | 33.234 -13.839 | | 1.00 43.78 | С |
| | ATOM | 1391 | | ILE | | 87 | 32.624 -13.331 | | 1.00 47.44 | С |
| 40 | MOTA | 1395 | | ILE | | 87 | 31.050 -13.435 | 15.795 | 1.00 39.53 | С |
| 40 | MOTA | 1399 | С | ILE | | 87 | 32.022 -15.517 | 18.062 | 1.00 43.32 | С |
| | MOTA | 1400 | 0 | ILE | | 87 | 31.287 -16.462 | | 1.00 44.61 | 0 |
| | MOTA | 1401 | N | PRO | Α | 88 | 32.120 -15.212 | 19.346 | 1.00 41.82 | N |
| | MOTA | 1402 | CA | PRO | Α | 88 | 31.440 -16.004 | 20.380 | 1.00 45.42 | C |
| | MOTA | 1404 | CB | PRO | Α | 88 | 31.311 -15.040 | 21.563 | 1.00 46.34 | С |
| 45 | MOTA | 1407 | CG | PRO | Α | 88 | 32.594 -14.147 | 21.446 | 1.00 46.41 | . C |
| | MOTA | 1410 | CD | PRO | A | 88 | 32.902 -14.107 | 19.925 | 1.00 46.82 | |
| | MOTA | 1413 | С | PRO | Α | 88 | 30.103 -16.508 | | 1.00 44.85 | C |
| | ATOM | 1414 | 0 | PRO | A | 88 | 29.867 -17.685 | 20.208 | | . O |
| | MOTA | 1415 | N | HIS | | 89 | 29.243 -15.692 | | 1.00 46.76 | N |
| 50 | MOTA | 1417 | CA | HIS | | 89 | 27.981 -16.214 | | 1.00 50.05 | C |
| | ATOM | 1419 | СВ | HIS | | 89 | 26.757 -15.526 | | 1.00 48.45 | Č |
| | ATOM | 1422 | CG | HIS | | 89 | 26.753 -15.317 | | 1.00 55.56 | C |
| | ATOM | 1423 | - | HIS | | 89 | 26.375 -16.302 | | 1.00 55.56 | N |
| | ATOM | 1425 | | HIS | | 89 | 26.460 -15.830 | | | |
| 55 | ATOM | 1427 | | | | • | | | 1.00 64.25 | c |
| ر ر | | | | HIS | | 89 | 26.878 -14.576 | • | 1.00 59.22 | N |
| | ATOM | 1429 | | HIS | | 89 | 27.065 -14.229 | | 1.00 56.69 | . C |
| | ATOM | 1431 | C | HIS | | 89 | 27.958 -15.966 | | 1.00 54.03 | С |
| | ATOM | 1432 | 0 | HIS | | 89 | 27.124 -15.179 | | 1.00 55.54 | 0 |
| 60 | ATOM | 1433 | N | GLY | | 90 . | 28.896 -16.606 | | 1.00 55.69 | N |
| 60 | ATOM | 1435 | CA | GLY | | 90 | 28.986 -16.585 | | 1.00 55.66 | С |
| | MOTA | 1438 | С | GLY | A | 90 | 29.407 -18.001 | 14.865 | 1.00 52.28 | С |
| | | | | | | | | | | |

| _ | | | _ | CTV A | 00 | 29.482 -18.847 15.746 1.00 62.08 | 0 |
|-----|--------|------|----------|----------------|----------|----------------------------------|-----|
| 5 | ATOM | 1439 | | GLY A | 90 | 29.704 -18.297 13.628 1.00 47.23 | N |
| | MOTA | 1440 | N | PRO A | 91 | 30.069 -19.664 13.308 1.00 47.93 | С |
| | ATOM | 1441 | CA | PRO A | 91 | 30.399 -19.586 11.830 1.00 49.04 | С |
| | MOTA | 1443 | CB | PRO A | 91 | 30.611 -18.114 11.561 1.00 45.67 | С |
| | ATOM | 1446 | CG | PRO A | 91 | 29.727 -17.419 12.456 1.00 48.30 | С |
| 10 | MOTA | 1449 | CD | PRO A | 91 | 31.248 -19.980 14.206 1.00 54.34 | С |
| | MOTA | 1452 | С | PRO A | 91 | 32.052 -19.090 14.448 1.00 56.82 | 0 |
| | MOTA | 1453 | 0 | PRO A | 91 | 31.343 -21.211 14.691 1.00 54.83 | N |
| | ATOM | 1454 | N | GLN A | 92 | 32.261 -21.569 15.765 1.00 55.86 | С |
| | MOTA | 1456 | CA | GLN A | 92 | 31.662 -22.754 16.503 1.00 60.18 | С |
| 15 | MOTA | 1458 | CB | GLN A | 92 | 30.322 -22.429 17.101 1.00 58.46 | С |
| | ATOM | 1461 | | GLN A | 92 | 30.470 -21.890 18.493 1.00 64.81 | С |
| | MOTA | 1464 | CD | GLN A | 92 | 30.847 -22.631 19.418 1.00 63.91 | 0 |
| | MOTA | 1465 | | GLN A | 92 | 30.178 -20.591 18.662 1.00 67.59 | . И |
| | MOTA | 1466 | | GLN A | 92 | 33.635 -21.950 15.325 1.00 56.89 | С |
| 20 | MOTA | 1469 | С | GLN A | 92 | 34.036 -23.111 15.411 1.00 62.48 | 0 |
| | ATOM | 1470 | 0 | GLN · A | 92 | 34.387 -20.961 14.897 1.00 55.14 | N |
| | ATOM | 1471 | N | VAL A | 93 | 35.629 -21.223 14.237 1.00 50.07 | · c |
| | ATOM | 1473 | CA | VAL A | 93 | 35.426 -21.112 12.760 1.00 51.39 | С |
| | MOTA | 1475 | CB. | VAL A | 93 | 34.450 -22.169 12.285 1.00 53.66 | , C |
| 25 | MOTA | 1477 | | VAL A | | 34.902 -19.715 12.424 1.00 53.54 | C |
| | MOTA | 1481 | | - VAL A | 93 | 36.605 -20.174 14.620 1.00 54.79 | С |
| | MOTA | 1485 | | VAL A | 93 | 36.303 -19.243 15.382 1.00 56.10 | 0 |
| | MOTA | 1486 | 0 | VAL A | 93 | 37.805 -20.303 14.089 1.00 53.29 | N |
| | MOTA | 1487 | N | THR A | 94 | 38.802 -19.378 14.467 1.00 52.14 | Ċ |
| 30 | ATOM . | 1489 | CA | THR A | 94 | 39.464 -19.960 15.690 1.00 53.16 | С |
| | ATOM | 1491 | CB | THR A | 94 | 38.506 -19.888 16.761 1.00 53.79 | О |
| | MOTA | 1493 | | THR A | 94. | 40.645 -19.093 16.197 1.00 56.24 | С |
| | ATOM | 1495 | | THR A | 94 | 39.688 -19.131 13.285 1.00 52.21 | С |
| | MOTA | 1499 | С | THR A | 94 | 40.148 -20.051 12.624 1.00 61.76 | 0 |
| 35 | MOTA | 1500 | 0 | THR A | 94 | 39.923 -17.867 12.993 1.00 51.10 | N. |
| | MOTA | 1501 | N | VAL A | 95 95 | 40.645 -17.543 11.772 1.00 48.01 | С |
| | MOTA | 1503 | CA | VAL A | 95 95 | 39.722 -16.862 10.706 1.00 43.19 | С |
| | MOTA | 1505 | | VAL A | 95 | 38.322 -17.270 10.858 1.00 37.56 | С |
| 40 | MOTA | 1507 | | L VAL A | 95 | 39.760 -15.377 10.824 1.00 47.32 | С |
| 40 | MOTA | 1511 | | 2 VAL A | | 41.736 -16.577 12.111 1.00 45.91 | С |
| | MOTA | 1515 | С | VAL A | | 41.608 -15.811 13.065 1.00 50.89 | 0 |
| | MOTA | 1516 | 0 | VAL A | | 42.814 -16.615 11.353 1.00 41.67 | N |
| | ATOM | 1517 | N | ARG A ARG A | | 43.788 -15.565 11.502 1.00 43.07 | С |
| 4 ~ | ATOM | 1519 | CA | ARG A | | 45.180 -16.043 11.235 1.00 41.47 | С |
| 45 | ATOM | 1521 | CB | ARG A | | 46.175 -14.982 11.546 1.00 41.13 | С |
| | ATOM | 1524 | CG CD | | _ | 47.579 -15.400 11.409 1.00 43.93 | C. |
| | MOTA | 1527 | | | | 48.156 -15.492 12.744 1.00 52.62 | N |
| | MOTA | 1530 | | | | 48.450 -16.621 13.334 1.00 56.20 | C |
| ~n. | MOTA | 1532 | | | | 48.233 -17.778 12.696 1.00 59.54 | N |
| 50 | MOTA. | 1533 | | 1. ARG A | | 48.965 -16.594 14.565 1.00 58.71 | N |
| | MOTA | 1536 | | 2 ARG A | | 43.441 -14.460 10.512 1.00 40.12 | С |
| | MOTA | 1539 | | ARG A | - | 43.081 -14.756 9.368 1.00 46.93 | . 0 |
| | MOTA | 1540 | | ARG A | | 43.539 -13.208 10.963 1.00 37.94 | N |
| | MOTA | 1541 | | ALA A | | 43.294 -12.033 10.119 1.00 40.48 | С |
| 55 | MOTA | 1543 | | | | 41.818 -11.575 10.255 1.00 40.89 | С |
| | MOTA | 1545 | | | | 44.193 -10.823 10.362 1.00 38.63 | С |
| | MOTA | 1549 | | ALA A | | 44.193 -10.673 11.393 1.00 40.23 | 0 |
| | MOTA | 1550 | | ALA A | | 44.208 -9.957 9.358 1.00 41.67 | N |
| | ATOM | 1551 | | ASN A | | 44.823 -8.658 9.427 1.00 39.41 | С |
| 60 | ATOM | 1553 | | | | 44.680 -7.992 8.094 1.00 42.95 | · С |
| | MOTA | 1555 | 5 CE | B ASN | 98 | 44.000 1.555 5.051 2.00 .5155 | |

| _ | | | | | _ | 0.0 | 45 476 | | 8.649 | 7.070 | 1 00 | 37.46 | | | С |
|------------|--------------|--------------|----------|-------|-----|------------|------------------|---|----------------|------------------|------|----------------|---|---|--------|
| 5 . | MOTA | 1558 | CG | ASN | | 98 | 45.476 | | 8.980 | 7.320 | | 37.53 | | | 0 |
| • | MOTA | 1559 | | ASN | | 98 | 46.593 44.915 | | -8.841 | 5.896 | | 52:61 | | | N |
| | MOTA | 1560 | | ASN | | 98 | 44.913 | | -7.799 | 10.369 | | 40.10 | | | С |
| | MOTA | 1563 | C | ASN | | 98 | 44.063 | | -7.864 | 10.434 | | 41.02 | | | 0 |
| | MOTA | 1564 | 0 | ASN | | 98 | 44.808 | | -6.962 | 11.089 | | 44.12 | | | N |
| 10 | MOTA | 1565 | N | ILE | | 99 | 44.198 | | -6.153 | 12.128 | | 44.32 | | | С |
| | MOTA | 1567 | CA | ILE | | 99 | | | -6.840 | 13.502 | | 41.75 | | | С |
| | MOTA | 1569 | CB | ILE | | 99 | 44.298 43.507 | | -8.127 | 13.511 | | 43.97 | | | С |
| | MOTA | 1571 | | ILE | | 99 | 43.588 | | -8.918 | 14.872 | | 48.22 | | | С |
| | MOTA | 1574 | | ILE | | 99 99 | 43.722 | | -5.928 | 14.602 | | 45.32 | | | С |
| 15 | ATOM | 1578 | | ILE | | 99 | 44.932 | | -4.844 | 12.154 | | 44.51 | | | С |
| | ATOM | 1582 | C | ILE | | 99 | 46.082 | | -4.777 | 11.783 | | 47.40 | | | 0 |
| | MOTA | 1583 | 0 | ILE | | | 44.252 | | -3.795 | 12.579 | | 45.36 | | | N |
| | ATOM | 1584 | | ALA | | | 44.880 | | -2.510 | 12.655 | | 41.65 | | | С |
| 00 | ATOM | 1586 | CA | | | 100 | 44.230 | | -1.553 | 11.762 | | 41.33 | | | C |
| 20 | ATOM | 1588 | CB | | | 100 | 44.732 | | -2.068 | 14.054 | | 42.41 | | | С |
| | ATOM | 1592 | C | | | 100 | 43.612 | | -1.861 | 14.531 | | 41.57 | | | 0 |
| | ATOM | 1593 | 0 | | | 101 | 45.865 | | -1.951 | 14.736 | | 40.77 | | | N |
| | ATOM | 1594 | N | | | 101 | 45.801 | | -1.461 | 16.066 | | 37.99 | | | С |
| 25 | ATOM | 1596 | CA CB | | | 101 | 46.907 | | -1.896 | 16.841 | | 44.45 | | | С |
| 25 | ATOM | 1598 1602 | СВ | | | 101 | 45.819 | | 0.007 | | | 41.73 | | | С |
| | MOTA | 1602 | ō | | | 101 | 46.801 | | 0.611 | 15.432 | 1.00 | 40.15 | | | 0 |
| | ATOM | 1604 | N | | | 102 | 44.656 | | 0.544 | 16.204 | | 42.71 | • | | N |
| | ATOM ATOM | 1604 | CA | | | 102 | 44.379 | | 1.911 | 16.241 | 1.00 | 39.72 | | | С |
| 30 | ATOM | 1608 | CB | | | 102 | 43.010 | | 2.009 | 16.549 | 1.00 | 44.46 | | | C |
| .50 | ATOM | 1610 | | ILE | | | 42.182 | | 1.767 | 15.321 | 1.00 | 43.48 | | | С |
| | ATOM | 1613 | | ILE | | | 40.76 | | 1.961 | 15.644 | | 40.40 | | | С |
| • | ATOM | 1617 | | ILE | | | 42.73 | 2 | 3.406 | 17.111 | | 48.29 | | | C |
| | ATOM | 1621 | | | | 102 | 45.02 | 4 | 2.449 | 17.452 | | 44.91 | | • | C . |
| 35 | ATOM | 1622 | | | | 102 | 44.77 | 7 | 1.856 | 18.522 | | 42.30 | | | 0 |
| ••. | ATOM | 1623 | N | THE | R A | 103 | 45.79 | | 3.544 | 17.257 | | 45.74 | | | N C |
| | ATOM | 1625 | CA | THE | RA | 103 | 46.58 | | 4.269 | 18.265 | | 48.02 | | | c |
| | ATOM | 1627 | CB | THE | A S | 103 | 48.11 | | 4.118 | 17.971 | | 48.61 | | | 0 |
| | ATOM | 1629 | OG 3 | L THE | RA | 103 | 48.36 | | 4.329 | 16.578 | | 53.38 | | | C |
| 40 | MOTA | 1631 | CG2 | | | 103 | 48.60 | | 2.733 | 18.209 | | 42.44 | | | c |
| | ATOM | 1635 | С | | | 103 | 46.29 | | 5.790 | 18.383 | | 48.94 | | | Ö |
| | MOTA | 1636 | 0 | | | 103 | 46.54 | | 6.358 | 19.407 | | 51.09 54.39 | | | N |
| | MOTA | 1637 | N | | | 104 | 45.80 | | 6.456 | 17.343 | | 56.21 | | | Ċ |
| | MOTA | 1639 | CA | | | 104 | 45.35 | | 7.855 | 17.474 | | 61.91 | | | c |
| 45 | MOTA | 1641 | CB | | | 104 | 46.40 | | 8.823 | 16.940 | | 66.58 | | | Č |
| | MOTA | 1644 | CG | | | 104 | 47.73 | | 8.206 | 16.593 15.758 | | 71.04 | | | Č |
| | MOTA | 1647 | ÇD | | | 104 | 48.59 | | 9.142 9.782 | | | 69.31 | | | ō |
| | ATOM | 1648 | | | | 104 | 48.03 | | | 16.037 | | 69.74 | | | 0 |
| | MOTA | 1649 | | | | 104 | 49.83 | | 9.228 | | | 53.27 | | | C |
| 50 | MOTA | 1650 | C | | | 104 | 44.06 | | 8.088 7.496 | | | 0 44.69 | | | 0 |
| | MOTA | 1651 | 0 | | | 104 | 43.89 | | 8.968 | | | 52.49 | | | N |
| | ATOM | 1652 | | | | 105 | 43.18 41.85 | | 9.143 | | | 0 54.80 | | | . с |
| | MOTA | 1654 | | | | 105 | 40.95 | | 8.049 | | | 0 53.62 | | | С |
| | MOTA | 1656 | | | | 105 | 41.28 | | 7.850 | | | 0 51.12 | | | 0 |
| 55 | ATOM | 1659 | | | | 105 | 41.13 | | 10.454 | | | 0 56.75 | | | С |
| | MOTA | 1661 | | | | 105 105 | 41.13 | | 11.077 | | | 0 57.71 | | | 0. |
| | ATOM | 1662 | | | | 105 | 40.30 | | 10.829 | | | 0 57.97 | | | N |
| | MOTA | 1663 | | | | 106 | 39.59 | | 12.109 | | | 0 57.67 | | | C |
| ۲۵ | MOTA | 1665 | | | | 106 | 40.3 | | 13.113 | | • | 0 60.33 | • | | С |
| 60 | | 1667 | CB | | | A 106 | 39.80 | | 14.562 | | | 0 66.40 | | | C |
| | MOTA | 1670 | , | . Ao | | | 33.0 | | | | | | | | |

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1.00 70.77
                                                                                       0
                                      39.308
                                               14.924
                                                       16.157
5
                  OD1 ASP A 106
            1671
     MOTA
                                                                1.00 70.32
                                               15.422
                                                        14.192
                  OD2 ASP A 106
                                      40.007
            1672
     MOTA
                                                                                       C
                                                                1.00 54.92
                                               11.950 15.391
                                      38.136
            1673
                  С
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     MOTA
                                                                                       O
                                                                1.00 46.42
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                                                        14.204
                                      37.824
                       ASP A 106
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                  N
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                                                                                       C
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                                                        16.136
                       LYS A 107
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            1677
                  CA
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     MOTA
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                                                        14.683
                                               15.570
            1685
                  CD
                       LYS A 107
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                                                                1.00 62.59
                                                                                       C
                                               16.997
                                                        15.235
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     MOTA
            1688
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                       LYS A 107
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                                                                1.00 61.25
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                                                        15.030
                       LYS A 107
            1691
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15
     ATOM
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                       LYS A 107
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            1695
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     MOTA
                                                                1.00 60.65
                                                                                       0
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                                               10.520
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                       LYS A 107
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                  CA
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                       PHE A 109
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                                                                 1.00 57.15
                                                                                       C
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                                                 4.114
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                                                                 1.00 52.57
                                                                                       С
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                       PHE A 109
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                   С
                                                                 1.00 50.58
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                                       34.087
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                                                                                        С
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                                                                 1.00 53.87
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                                                                                        С
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                                                 7.492
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                        ILE A 110
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                   С
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                                                                 1.00 47.53
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                                                 6.355
             1755
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                        ILE A 110
     ATOM
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                        GLN A 111
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                   CB
50
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     ATOM
                                                         26.046 1.00 62.67
                                                                                        C
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                   CG
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                        GLN A 111
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                                                11.816
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                   NE2 GLN A 111
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      ATOM
                                                                                        С
                                                                 1.00 57.17
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                                       29.816
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                        GLN A 111
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      MOTA
                                                 7.829
                                                         23.730
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                        GLN A 111
      MOTA
             1772
                   0
                                                                                        N
                                        30.012
                                                 6.560
                                                         25.043
                                                                 1.00 54.22
                        GLY A 112
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                   N
      MOTA
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                                                 5.803
             1775
                   CA
      MOTA
                                                         24.486 1.00 58.44
                                                  4.937
                                        28.279
             1778
                   С
                        GLY A 112
      MOTA
                                                  4.561
                                                         24.538 1.00 61.06
                                        27.109
                        GLY A 112
 60
             1779
                   0
      MOTA
                                        29.083
                                                         23.501 1.00 61.23
                                                  4.599
             1780
                    N
                        SER A 113
      MOTA
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| | | 1782 CA SER A 113 | 28.603 3.762 22.424 1.00 58.94 C |
|-----|-------|--------------------|-----------------------------------|
| 5 | | 117 | 29 408 4.080 21.174 1.00 60.39 |
| | | | 30 773 4 180 21.514 1.00 59.53 |
| | | | 29 687 2 272 22.768 1.00 54.01 |
| | | | 27 891 1.528 22.279 1.00 53.79 |
| | | | 29 642 1 879 23.613 1.00 48.58 N |
| 10 | | | 29 882 0.505 24.026 1.00 47.72 C |
| | | 1793 CA ASN A 114 | 28 660 -0.222 24.481 1.00 52.15 |
| | MOTA | 1795 CB ASN A 114 | 29 015 -1.423 25.395 1.00 61.51 |
| | | 1798 CG ASN A 114 | 20 436 -1 259 26.544 1.00 64.39 |
| | ATOM | 1799 OD1 ASN A 114 | 29 867 -2 632 24.867 1.00 65.83 N |
| 15 | MOTA | 1800 ND2 ASN A 114 | 30.664 -0.364 23.028 1.00 50.29 C |
| | MOTA | 1803 C ASN A 114 | 30 981 -1 544 23.314 1.00 51.67 |
| | MOTA | 1804 O ASN A 114 | 31 014 0 204 21 871 1.00 48.89 N |
| , | MOTA | 1805 N TRP A 115 | 31.022 -0.536 20.929 1.00 46.17 C |
| | MOTA | 1807 CA TRP A 115 | 31.344 -0.530 19.518 1.00 42.77 C |
| 20 | MOTA | 1809 CB TRP A 115 | 20 007 0 748 18.828 1.00 39.20 C |
| | MOTA | 1812 CG TRP A 115 | 20.722 1.338 18.787 1.00 35.62 C |
| | ATOM | 1813 CD1 TRP A 115 | 23.722 1.00 1.00 36 54 N |
| | MOTA | 1815 NE1 TRP A 115 | 29.102 |
| | MOTA | 1817 CE2 TRP A 115 | 51.055 |
| 25 | ATOM | 1818 CD2 TRP A 115 | 31.703 1.703 1.00 37 81 C |
| | MOTA | 1819 CE3 TRP A 115 | 33.132 2.016 1 00 33 70 |
| | MOTA | 1821 CZ3 TRP A 115 | 33.001 |
| | ATOM | 1823 CH2 TRP A 115 | 32.324 1 00 40 37 C |
| | ATOM | 1825 CZ2 TRP A 115 | 31.007 |
| 30 | MOTA | 1827 C TRP A 115 | 01 772 1 00 54 94 |
| 50 | ATOM | 1828 O TRP A 115 | 33.341 N |
| | ATOM | 1829 N GLU A 116 | J4.204 0 1 00 50 10 |
| | MOTA | 1831 CA GLU A 116 | 35.607 -0.389 20.433 1.00 54 65 |
| | ATOM | 1833 CB GLU A 116 | 36.192 -1.236 21.600 1.00 57.18 C |
| 35 | ATOM | 1836 CG GLU A 116 | 35.916 -0.715 22.990 1.00 50.55 C |
| 33 | MOTA | 1839 CD GLU A 116 | 34.9/9 =1.591 25.000 1.00 63.96 |
| | MOTA | 1840 OE1 GLU A 116 | 34.203 |
| | MOTA | 1841 OE2 GLU A 116 | 34.544 C |
| | MOTA | 1842 C GLU A 116 | 36.444 -0.607 19.210 1.00 35.00 |
| 40 | ATOM | 1843 O GLU A 116 | 37.686 -0.501 19.227 1.00 40.13 |
| -10 | ATOM | 1844 N. GLY A 117 | 55.752 16.000 1.00 47.29 C |
| | ATOM | 1846 CA GLY A 117 | 36.435 -1.222 16.502 1.00 17.00 C |
| • | ATOM | 1849 C GLY A 117 | 35.469 -1.364 13.730 1.00 17.00 |
| | ATOM | 1850 O GLY A 117 | 34.257 -1.112 15.756 1.00 50.00 |
| 45 | | 1851 N ILE A 118 | 35.999 -1.781 14.041 1.00 18.00 C |
| 43 | ATOM | 1853 CA ILE A 118 | 35.113 -1.752 13.333 1.00 33.44 |
| | ATOM | 1855 CB ILE A 118 | 35.323 -0.489 12.671 1.00 33.55 |
| | ATOM | 1857 CG1 ILE A 118 | 34.441 -0.331 11.053 1.00 30 06 |
| | ATOM | 1860 CD1 ILE A 118 | 34.304 1.118 11.233 1.00 41 01 |
| 50 | | 1864 CG2 ILE A 118 | 36.669 -0.442 12.300 1.30 |
| 30 | | 1868 C ILE A 118 | 35.465 -2.905 12.000 1.00 35.00 |
| - | MOTA | 1869 O ILE A 118 | 36.608 -3.210 12.402 1.00 12.10 |
| | ATOM. | 1870 N LEU A 119 | 34.445 -3.566 12.175 1.00 39.01 |
| | ATOM | | 34.628 -4.621 11.269 1.00 38.51 |
| | ATOM | | 33.759 -5.772 11.693 1.00 39.97 |
| 55 | | | 33.969 -6.973 10.812 1.00 40.38 |
| | MOTA | | 35.433 -7.445 10.870 1.00 37.17 |
| | ATOM | | 33.036 -8.028 11.273 1.00 42.73 |
| | MOTA | 110 | 34 151 -4 097 9.953 1.00 38.40 |
| | MOTA | 110 | 32 965 -3 923 9.771 1.00 43.72 |
| 60 | | - 100 | 35.059 -3.794 9.039 1.00 40.26 N |
| | ATOM | 1889 N GLY A 120 | |

| 5 | ATOM | 1891 | CA | GLY A | 120 | | 34.655 | -3.388 | 7.696 | 1.00 37.27 | | | С |
|-------------|------|------|-----|-------|-----|----|--------|--------|--------|------------|-----|---|------------|
| | ATOM | 1894 | C · | GLY A | | | 34.278 | -4.619 | 6.920 | 1.00 35.23 | | | С |
| | ATOM | 1895 | 0 | GLY A | | • | 35.044 | -5.538 | 6.888 | 1.00 41.95 | | , | 0 |
| | ATOM | 1896 | N | LEU A | 121 | | 33.116 | -4.697 | 6.293 | 1.00 40.05 | | | N |
| | ATOM | 1898 | CA | LEU A | 121 | | 32.866 | -5.891 | 5.473 | 1.00 34.58 | | | С |
| 10 | ATOM | 1900 | CB | LEU A | 121 | | 31.626 | -6.622 | 5.917 | 1.00 35.45 | | | С |
| •- | ATOM | 1903 | CG | LEU A | | | 31.436 | -6.831 | 7.393 | 1.00 31.35 | | | С |
| | ATOM | 1905 | | LEU A | | | 29,950 | -6.863 | 7.687 | 1.00 28.15 | | | С |
| | ATOM | 1909 | | LEU A | | | 32.124 | -8.105 | 7.719 | 1.00 28.77 | | | С |
| | ATOM | 1913 | С | LEU A | | | 32.704 | -5.635 | 3.984 | 1.00 37.29 | | | C |
| 15 | ATOM | 1914 | 0 | LEU A | | ٠. | 32.158 | -6.483 | 3.267 | 1.00 42.02 | | | 0 |
| | ATOM | 1915 | N | ALA A | - | | 33.145 | -4.505 | 3.469 | 1.00 36.05 | | | N |
| | ATOM | 1917 | CA | ALA A | | | 33.084 | -4.404 | 2.029 | 1.00 39.37 | • | | С |
| | ATOM | 1919 | СВ | ALA A | | | 32.974 | -3.039 | 1.593 | 1.00 40.38 | • , | | С |
| • | ATOM | 1923 | С | ALA A | | | 34.289 | -5.090 | 1.398 | 1.00 41.97 | | | С |
| 20 | ATOM | 1924 | Ō | ALA A | | | 35.020 | -5.841 | 2.046 | 1.00 40.99 | | | 0 |
| | ATOM | 1925 | N | TYR A | | | 34.486 | -4.796 | 0.124 | 1.00 43.02 | | | N |
| | ATOM | 1927 | CA | TYR A | | | 35.423 | -5.522 | -0.690 | 1.00 40.35 | | | С |
| | ATOM | 1929 | СВ | TYR A | | | 34.904 | -5.453 | | 1.00 38.74 | | | С |
| | ATOM | 1932 | CG | TYR A | | | 33.687 | -6.306 | -2.361 | 1.00 41.64 | | | С |
| 25 | ATOM | 1933 | | TYR A | | | 32.453 | -5.755 | -2.557 | 1.00 39.22 | | | Ċ |
| 20 | ATOM | 1935 | | TYR A | | | 31.352 | -6.564 | -2.824 | 1.00 34.66 | | | C |
| | ATOM | 1937 | CZ | TYR A | | | 31.487 | -7.899 | -2.896 | 1.00 36.31 | | | C |
| | ATOM | 1938 | OH | TYR A | | | 30.392 | -8.724 | -3.167 | 1.00 43.22 | | | 0 |
| | ATOM | 1940 | | TYR A | | | 32.711 | -8.459 | -2.706 | 1.00 43.43 | | | Č |
| 30 | ATOM | 1942 | | TYR A | | | 33.788 | -7.686 | -2.443 | 1.00 43.16 | | | C |
| 50 | ATOM | 1944 | C | TYR A | | | 36.758 | -4.856 | -0.586 | 1.00 43.96 | | | Ċ |
| | ATOM | 1945 | ŏ | TYR A | | | 36.831 | -3.746 | -0.094 | 1.00 43.08 | | | ō |
| • | ATOM | 1946 | N | ALA A | | | 37.810 | -5.509 | -1.063 | 1.00 46.53 | | | N |
| | ATOM | 1948 | CA | ALA A | | | 39.194 | -5.021 | -0.894 | 1.00 45.27 | | | C |
| 35 | ATOM | 1950 | СВ | ALA A | | | 40.163 | -6.124 | -1.311 | 1.00 45.24 | | • | Ċ |
| 55 . | ATOM | 1954 | c | ALA A | | | 39.597 | -3.728 | -1.616 | 1.00 47.88 | | | C |
| • | ATOM | 1955 | ō | ALA A | | | 40.511 | -2.999 | -1.159 | 1.00 47.35 | | | 0 |
| | ATOM | 1956 | N | GLU A | | | 38.950 | -3.438 | -2.735 | 1.00 46.72 | | | N |
| | ATOM | 1958 | CA | GLU A | | | 39.399 | -2.342 | -3.574 | 1.00 46.92 | | | С |
| 40 | ATOM | 1960 | СВ | GLU A | | | 38.461 | -2.169 | -4.774 | 1.00 49.10 | | | С |
| • • | ATOM | 1963 | CG | GLU A | | • | 38.608 | -0.831 | -5.492 | 1.00 55.04 | - | | С |
| | ATOM | 1966 | CD | GLU A | | | 37.786 | -0.739 | -6.766 | 1.00 58.92 | | | С |
| | ATOM | 1967 | | GLU A | | | 37.095 | -1.730 | -7.135 | 1.00 59.91 | | | 0 |
| | ATOM | 1968 | | GLU A | | | 37.819 | 0.355 | -7.409 | 1.00 68.22 | | | 0 |
| 45 | ATOM | 1969 | | GLU A | | | 39.511 | -1.074 | -2.753 | 1.00 49.28 | | | С |
| | MOTA | 1970 | ō | GLU A | | | 40.486 | -0.298 | -2.858 | 1.00 51.06 | | | 0 |
| | ATOM | 1971 | N | ILE A | | | 38.521 | -0.843 | -1.908 | 1.00 46.11 | | | N |
| | ATOM | 1973 | CA | ILE A | | | 38.561 | | -1.157 | 1.00 43.32 | | | С |
| | ATOM | 1975 | СВ | ILE A | | | 37.142 | 0.953 | -0.961 | 1.00 47.04 | | | С |
| 50 | ATOM | 1977 | | ILE A | | | 36.254 | 0.022 | -0.122 | 1.00 44.04 | | | С |
| 50 | ATOM | 1980 | | ILE A | | | 34.965 | 0.642 | 0.383 | 1.00 50.45 | | | C |
| .* | ATOM | 1984 | | ILE A | | | 36.539 | 1.274 | -2.351 | 1.00 46.90 | | - | C |
| • | ATOM | 1988 | C | ILE A | | | 39.288 | 0,228 | 0.142 | 1.00 44.66 | | | Ċ. |
| • | ATOM | 1989 | ŏ | ILE A | | | 39.146 | 1.085 | 1.007 | 1.00 48.22 | | | ō |
| 55 | ATOM | 1990 | N | ALA A | | | 40.093 | -0.808 | | 1.00 44.81 | | | N |
| J.J | MOTA | 1992 | CA | ALA A | | • | 40.788 | -0.914 | 1.580 | 1.00 48.39 | | | C |
| | ATOM | 1994 | CB | ALA A | | | 40.982 | -2.321 | 1.937 | 1.00 50.81 | | | c |
| | ATOM | 1998 | С | ALA A | | | 42.119 | -0.200 | 1.613 | 1.00 52.76 | | , | C |
| | ATOM | 1999 | Ö | ALA A | | | 42.119 | 0.145 | 0.574 | 1.00 59.40 | | | Ö |
| 60 | MOTA | 2000 | ·N | ARG A | | | 42.591 | 0.143 | 2.838 | 1.00 51.36 | | | N |
| JU | MOTA | 2002 | CA | ARG A | | | 43.783 | 0.715 | 3.064 | 1.00 51.80 | | | Ċ. |
| | HIOU | 2002 | Or1 | and n | 120 | | 23.103 | 0.713 | 5.003 | 2.00 02.00 | | | - . |

| | | | -50 3 100 | | 43.430 | 1.900 | 3.897 | 1.00 56.05 | | (| С |
|------|-------|---------|---------------|-----|--------|----------|--------|------------|----|---|------|
| 5 | MOTA | 2004 CB | ARG A 128 | | 42.275 | 2.626 | | 1.00 59.64 | | | С |
| | MOTA | 2007 CG | ARG A 128 | | 42.275 | 2.934 | 1.917 | 1.00 69.11 | * | | С |
| | MOTA | 2010 CD | ARG A 128 | | 41.482 | 4.108 | 1.663 | 1.00 79.76 | • | | N |
| | MOTA | 2013 NE | ARG A 128 | | | 5.318 | 2.018 | 1.00 81.91 | | | С |
| | ATOM | 2015 CZ | ARG A 128 | | 41.839 | 5.508 | 2.630 | 1.00 80.28 | | | N |
| 10 | MOTA | 2016 NH | 1 ARG A 128 | | 43.001 | | 1.759 | 1.00 87.99 | | | N |
| | ATOM | 2019 NH | 2 ARG A 128 | | 41.039 | 6.335 | 3.828 | 1.00 51.97 | | | С |
| | MOTA | 2022 C | ARG A 128 | | | -0.135 | 4.689 | 1.00 49.70 | | | 0 |
| | ATOM | 2023 O | ARG A 128 | | | -0.987 | 3.544 | 1.00 44.07 | | | N |
| | MOTA | 2024 N | PRO A 129 | | 46.129 | 0.076 | | 1.00 39.23 | | | С |
| 15 | MOTA | 2025 CA | | : . | 46.636 | 1.004 | 2.539 | 1.00 39.26 | | | С |
| 15 | ATOM | 2027 CB | | | 48.105 | 0.812 | 2.595 | 1.00 39.20 | | | |
| | MOTA | 2030 CG | PRO A 129 | | 48.386 | -0.019 | 3.710 | 1.00 44.03 | | | Č |
| | ATOM | 2033 CD | PRO A 129 | | 47.196 | -0.642 | 4.242 | | | • | c |
| • | ATOM | 2036 C | PRO A 129 | | 46.254 | 0.674 | 1.113 | 1.00 45.48 | | | o |
| 20 | MOTA | 2037 0 | PRO A 129 | | 46.153 | 1.658 | 0.336 | 1.00 46.05 | | | N |
| 20 | | 2038 N | ASP A 130 | | 46.101 | -0.637 | 0.783 | 1.00 46.52 | | | C |
| | MOTA | 2040 CA | | | 45.574 | | -0.520 | 1.00 47.07 | | | C |
| | MOTA | 2040 CB | | | 46.563 | | -1.653 | 1.00 52.49 | | | |
| | ATOM | 2042 CD | | | 47.874 | -1.365 | -1.520 | 1.00 58.99 | | | C |
| 0.5 | MOTA | | 1 ASP A 130 | | 48.849 | -0.917 | -2.187 | 1.00 66.76 | | | 0 , |
| 25 | MOTA | | 2 ASP A 130 | • | 48.023 | -2.366 | -0.794 | 1.00 64.97 | ٠. | | 0 . |
| | MOTA | | ASP A 130 | | 44.937 | -2.355 | -0.652 | 1.00 44.59 | | | С |
| | MOTA | 2048 C | ASP A 130 | | 44.877 | -3.167 | 0.272 | 1.00 50.22 | | | 0 |
| 1. | MOTA | 2049 0 | ASP A 130 | | 44.443 | -2.606 | -1.834 | 1.00 41.96 | | | N |
| | ATOM. | 2050 N | | | 43.679 | -3.802 | -2.024 | 1.00 45.38 | • | | C |
| 30 | MOTA | | A ASP A 131 | | 43.076 | -3.828 | -3.427 | 1.00 45.37 | | • | C |
| | MOTA | 2054 CI | | | 44.106 | -4.043 | -4.476 | 1.00 54.14 | | | С |
| | MOTA | | S ASP A 131 | | 45.130 | -4.692 | -4.143 | 1.00 60.53 | | | 0 |
| | MOTA | | D1 ASP A 131 | | 43.130 | -3.593 | -5.648 | 1.00 58.51 | | | О |
| | MOTA | | D2 ASP A 131 | | | -5.085 | -1.770 | 1.00 41.04 | | | С |
| 35 | MOTA | 2060 C | 404 | | 44.437 | -6.123 | -2.065 | 1.00 49.55 | | | 0 |
| | MOTA | 2061 O | | | 43.912 | -5.050 | -1.247 | 1.00 39.75 | | | N |
| | MOTA | 2062 N | | • | 45.645 | -6.304 | -1.002 | 1.00 45.06 | | • | С |
| | MOTA | 2064 C. | | | 46.409 | -6.174 | -1.605 | 1.00 43.25 | | | C |
| | ATOM | 2066 C | | | 47.788 | -4.995 | -1.060 | 1.00 53.72 | | | 0 |
| 40 | ATOM | 2069 O | | | 48.375 | | 0.489 | 1.00 41.26 | | | С |
| | MOTA | 2071 C | | | 46.582 | -6.591 | 0.403 | 1.00 52.36 | | | 0 |
| | MOTA | 2072 0 | | | 47.588 | -7.115 | 1.242 | 1.00 43.42 | | | N |
| • | ATOM | 2073 N | | | 45.584 | -6.162 | 2.687 | | | | Ç |
| | MOTA | 2075 C | A LEU A 133 | | 45.558 | -6.239 | | | | | C |
| 45 | ATOM | 2077 C | B LEU A 133 | | 45.773 | -4.923 | 3.419 | 1.00 41.79 | | | С |
| | MOTA | 2080 C | G LEU A 133 | | 45.518 | -5.228 | | | | | C |
| | ATOM | 2082 | D1 LEU A 133 | | 46.832 | -5.498 | 5.559 | | | | Ç |
| | ATOM | 2086 | D2 LEU A 133 | | 44.771 | -4.164 | 5.716 | 1.00 44.00 | | | č |
| | ATOM | 2090 | | | | 6.677 | 2.929 | 1.00 47.10 | | | ŏ |
| 50 | ATOM | | LEU A 133 | | 43.330 | -5.956 | 3.439 | | | | N |
| . 50 | | | N GLU A 134 | | 43.977 | | 2.510 | | | | |
| | MOTA | | CA GLU A 134 | | 42.777 | -8.725 | 2.630 | 1.00 48.06 | | - | C |
| | MOTA | | CB GLU A 134 | | 43.241 | -10.178 | 2.777 | | | | C |
| | MOTA | | CG GLU A 134 | | 42.169 | -11.212 | 3.013 | | | | . C |
| | MOTA | | CD GLU A 134 | • | 42.689 | -12.623 | 2.75 | | | | C |
| 55 | | | OE1 GLU A 134 | | 42 980 | -12.874 | | 1.00 55.42 | ٠. | | 0 |
| | MOTA | | | | 42.917 | -13.448 | | | | | . 0 |
| | MOTA | | OE2 GLU A 134 | | 41.837 | | 3.78 | | ٠ | | , c |
| | MOTA | | C GLU A 134 | | 42.23 | | | | | | ⊹, 0 |
| | MOTA | | O GLU A 134 | | 42.23 | | | | • | | N |
| - 60 | MOTA | | N PRO A 135 | | | | | | • | | . C |
| | MOTA | 2108 | CA PRO A 135 | | 39.53 | L -0.093 | | | | | |

| 5 . | ATOM | 2110 | СВ | PRO | Α | 135 | | 38.3 | 55 | -7.629 | 3.597 | 1.00 | 37.44 | | С |
|------|------|------|-----|-----|---|-----|---|------|----|---------|--------|------|-------|---|-----|
| | MOTA | 2113 | CG | PRO | A | 135 | | 38.8 | 53 | -7.363 | 2.237 | 1.00 | 40.45 | | C |
| | ATOM | 2116 | CD | PRO | | | | 40.0 | 71 | -8.171 | 2.068 | 1.00 | 42.71 | | C |
| | ATOM | 2119 | C | | | 135 | | 39.1 | | -9.353 | 5.269 | 1.00 | 36.44 | | С |
| | ATOM | 2120 | ō | PRO | | | | | | -10.450 | 4.767 | 1.00 | 34.69 | | 0 |
| - 10 | ATOM | 2121 | N | PHE | | | | 38.6 | | -9.163 | 6.505 | | 35.67 | | N |
| 10 | ATOM | 2123 | CA | PHE | | | | | | -10.241 | 7.427 | 1.00 | 31.72 | | С |
| | ATOM | 2125 | СВ | PHE | | | | | | -9.676 | 8.625 | 1.00 | 27.91 | | С |
| | ATOM | 2128 | CG | PHE | | | | | | -10.727 | 9.517 | | 28.87 | | С |
| | ATOM | 2129 | | PHE | | | | | | -11.301 | 10.550 | | 32.96 | | С |
| 15 | ATOM | 2131 | | PHE | | | | | | -12.267 | 11.382 | | 33.11 | | С |
| 15 | ATOM | 2133 | CZ | PHE | | | | | | -12.663 | 11.195 | 1.00 | 33.91 | | С |
| | ATOM | 2135 | | PHE | | | | | | -12.111 | 10.175 | | 36.07 | | С |
| | ATOM | 2137 | | PHE | | | | | | -11.137 | 9.333 | | 37.92 | | C. |
| • | ATOM | 2139 | | PHE | | | | | | -11.218 | 6.753 | | 35.77 | | С |
| 20 | ATOM | 2140 | ŏ | PHE | | | | | | -12.376 | 6.668 | | 45.44 | • | 0 |
| 20 | ATOM | 2141 | N | PHE | | | | | | -10.778 | 6.261 | | 40.56 | | N |
| | ATOM | 2143 | CA | PHE | | | | | | -11.754 | 5.677 | | 43.42 | | C. |
| | ATOM | 2145 | CB | PHE | | | | | | -11.132 | 5.014 | | 43.68 | | C |
| | ATOM | 2148 | | PHE | | | | | | -12.067 | 5.028 | | 41.41 | | C |
| 25 | ATOM | 2149 | | PHE | | | | | | -12.231 | 6.160 | | 38.90 | | C |
| 23 | ATOM | 2151 | | PHE | | | | | | -13.107 | 6.179 | | 36.47 | | С |
| • | ATOM | 2153 | CZ | PHE | | | | | | -13.824 | 5.087 | | 36.88 | | C |
| | ATOM | 2155 | | PHE | | | | | | -13.682 | 3.958 | | 39.68 | | C |
| | ATOM | 2157 | | PHE | | | | | | -12.809 | 3.922 | | 43.99 | | Ċ |
| 30 | ATOM | 2159 | | PHE | | | | | | -12.571 | 4.704 | | 43.89 | | c |
| , 30 | ATOM | 2160 | ō | PHE | | | | | | -13.774 | 4.828 | | 41.80 | | o · |
| | ATOM | 2161 | N | ASP | | | • | | | -11.904 | 3.762 | | 47.91 | | N |
| | ATOM | 2163 | CA | ASP | | | | | | -12.581 | 2.776 | | 47.51 | | C |
| | ATOM | 2165 | CB | ASP | | | | | | -11.632 | 2.142 | | 51.24 | | c |
| 35 | | 2168 | CG. | ASP | | | | | | -11.344 | 0.725 | | 54.56 | | Č |
| 33 | ATOM | 2169 | | ASP | | | | | | -12.027 | -0.179 | • | 66.25 | | 0 |
| | ATOM | 2170 | | ASP | | | | | | -10.434 | 0.419 | | 57.65 | | 0 |
| | ATOM | 2171 | C | ASP | | | | | | -13.684 | 3.394 | | 47.78 | | C |
| | ATOM | 2172 | 0 | ASP | | | | | | -14.788 | 2.886 | | 57.75 | | 0 |
| 40 | ATOM | 2173 | N | | | 139 | | | | -13.385 | 4.482 | | 46.16 | | N |
| | ATOM | 2175 | CA | | | 139 | | | | -14.405 | 5.145 | | 42.31 | | С |
| | ATOM | 2177 | СВ | | | 139 | | | | -13.740 | 6.204 | | 42.45 | | С |
| | ATOM | 2180 | OG | | | 139 | | | | -12.754 | 5.615 | | 35.20 | | 0 |
| | ATOM | 2182 | C | | | 139 | | | | -15.421 | 5.797 | | 43.01 | | С |
| 45 | ATOM | 2183 | ō | | | 139 | | | | -16.570 | 5.891 | | 42.82 | | 0 |
| | ATOM | 2184 | N | | | 140 | | | | -15.016 | 6.279 | | 50.41 | | N |
| - | ATOM | 2186 | CA | | | 140 | | | | -15.973 | 7.006 | | 46.59 | | С |
| • | ATOM | 2188 | | LEU | | | | | | -15.302 | 7.483 | | | | С |
| | ATOM | 2191 | CG | | | 140 | | | | -16.175 | 8.248 | | 54.03 | | С |
| 50 | ATOM | 2193 | | LEU | | | | | | -16.828 | 9.380 | | 56.74 | | Ċ |
| 50 | ATOM | 2197 | | LEU | | | | | | -15.327 | 8.755 | | 52.27 | | С |
| . ' | ATOM | 2201 | C | | | 140 | | | | -17.129 | 6.139 | | 48.27 | | С |
| | MOTA | 2202 | ŏ | | | 140 | | | | -18.231 | 6.649 | | 48.66 | | 0 |
| | ATOM | 2203 | N | | | 141 | | | | -16.868 | 4.833 | | 46.25 | | N |
| 55 | ATOM | 2205 | | VAL | | | • | | | -17.909 | 3.873 | | 48.65 | | C |
| 73 | ATOM | 2207 | CB | | | 141 | | | | -17.376 | 2.644 | ** | 49.70 | | Ċ |
| | ATOM | 2209 | | | | 141 | | | | -18.555 | 1.662 | | 50.68 | | č |
| | ATOM | 2213 | | VAL | | | | | | -16.801 | 3.069 | | 50.47 | | Č |
| | ATOM | 2217 | C | | | 141 | | | | -18.777 | 3.388 | | 54.04 | | Ċ |
| 60 | ATOM | 2218 | Ö | | | 141 | • | | | -19.989 | 3.354 | | 62.33 | | ō |
| vv | ATOM | 2219 | N | | | 142 | | | | -18.195 | 3.009 | | 53.50 | | N |
| | WIOH | 6473 | 14 | | | | | 50 | | 10.173 | | | 55.50 | | |

| | | | _ | |
|------|--------------|----------------------|------------------------------------|----|
| | | | 39.497 -18.997 2.510 1.00 51.72 C | |
| 5 | MOTA | 2221 CA LYS A 142 | 10 700 10 173 2 027 1.00 51.19 | |
| - | MOTA | 2223 CB LYS A 142 | 10.466 -16.996 1.006 1.00 55.43 | |
| | MOTA | 2226 CG LYS A 142 | 41 700 -16 385 0.423 1.00 59.35 | |
| | ATOM | 2229 CD LYS A 142 | 11.737 -15 659 -0.919 1.00 61.18 | |
| | MOTA | 2232 CE LYS A 142 | 10 012 15 043 -0.953 1.00 69.14 N | |
| 10 | MOTA | 2235 NZ LYS A 142 | 20.212 10.012 3.571 1.00 52.97 C | |
| 10 | ATOM | 2239 C LYS A 142 | 39.970 20.002 3.211 1.00 55.66 | |
| | ATOM | 2240 O LYS A 142 | 40.045 20.500 A 851 1.00 47.49 N | |
| | ATOM | 2241 N GLN A 143 | 39.634 15.666 5 937 1.00 47.98 | |
| | ATOM | 2243 CA GLN A 143 | 40.165 20.000 7 7 058 1.00 44.95 C | |
| 15 | ATOM | 2245 CB GLN A 143 | 40.616 15.77 | |
| 1.5 | ATOM | 2248 CG GLN A 143 | 42.100 13.200 7 691 1.00 52.26 | |
| | MOTA | 2251 CD GLN A 143 | 42.522 17.552 8 918 1.00 55.17 | |
| | MOTA | 2252 OE1 GLN A 143 | 42.540 16.702 7.081 1.00 48.24 | |
| • | MOTA | 2253 NE2 GLN A 143 | 44.101 101.00 | Ι, |
| 20 | ATOM | 2256 C GLN A 143 | 33.130 21.3° (| 0 |
| 20 | MOTA | 2257 O GLN A 143 | 39.303 22.22 | N |
| • | MOTA | 2258 N THR A 144 | 31.303 21.010 | С |
| | MOTA | 2260 CA THR A 144 | 30.313 22 | С |
| | ATOM | 2262 CB THR A 144 | 30.223 21.73 | 0 |
| 25 | ATOM | 2264 OG1 THR A 144 | 33.131 20.30 | С |
| 23 | ATOM | 2266 CG2 THR A 144 | 31.139 20.100 | С |
| | ATOM | 2270 C THR A 144 | 33.073 22.73 | 0 |
| | MOTA | 2271 O THR A 144 | 30.0/1 22:300 | N |
| | ATOM | 2272 N HIS A 145 | 34,112 23,302 | С |
| 20 | | 2274 CA HIS A 145 | 33,700 23,700 | С |
| 30 | MOTA MOTA | 2276 CB HIS A 145 | 33,313 23,223 | С |
| | | 2279 CG HIS A 145 | 34.393 20.200 | N |
| | MOTA | 2280 ND1 HIS A 145 | 33.032 20.01 | С |
| | MOTA | 2282 CE1 HIS A 145 | 33.300 27.00 | N |
| 25 | MOTA | 2284 NE2 HIS A 145 | 35.002 21.000 | С |
| - 35 | MOTA | 2286 CD2 HIS A 145 | 34.09/ 2000 | С |
| | ATOM | 2288 C HIS A 145 | 32.307 22.020 | 0 |
| | MOTA | 2289 O HIS A 145 | 31.392 23.000 | N |
| | MOTA | 2290 N VAL A 146 | 34.013 21.120 | С |
| 40 | MOTA | 2292 CA VAL A 146 | 31.339 20.01 | С |
| - 40 | | 2294 CB VAL A 146 | 31.049 13.002 | С |
| | MOTA | A COL 1737 3 146 | 30.713 10.723 | С |
| | MOTA | CCC VAT A 146 | 36.122 -20.11 | C |
| | ATOM | TINT N 146 | 31.24/ 20.302 | 0 |
| 4.5 | ATOM | 0 MAT N 1/6 | 32.110 13.100 | N |
| 45 | | DDO 7 147 | 30.023 20 | C |
| | ATOM | 222 CN DDO A 147 | 29.613 -19.931 2.649 1.00 36.28 | Ç |
| | ATOM | on DDO 7 147 | 28.139 -20.275 2.599 1.00 36.61 | Č |
| | ATOM | 20 DDO 7 147 | 28.062 -21.485 3.451 1.00 37.97 | č |
| | MOTA | an nno n 147 | 28.953 -21.213 4.609 1.00 37.03 | c |
| . 50 | | | 29.793 -18.397 2.535 1.00 30.02 | o |
| • | 1OTA | 100 A 147 | 29.688 -17.668 3.519 1.00 36.50 | N. |
| | ATO | 1 201 7 140 | 30.042 -17.926 1.318 1.00 37.03 | C |
| ÷ | ATO | CN 7 148 | 30 370 -16.536 1.041 1.00 35.69 | C |
| | OTA | OD DCN N 1/18 | 31 113 -16.480 -0.280 1.00 35.18 | |
| 5. | 5 ATO | | 21 701 -15 208 -0.460 1.00 38.29 | C |
| | OTA | | 21 000 -14 492 0.507 1.00 48.87 | 0 |
| | ATO | | 22 170 -14 888 -1.683 1.00 43.21 | N |
| | OTA | M 2329 ND2 ASN A 148 | 20 194 -15 584 0.950 1.00 37.44 | C |
| | ATO | M 2332 C ASN A 146 | 28 928 -14.994 -0.110 1.00 34.38 | 0 |
| . 6 | OTA 0 | M 2333 O ASN A 148 | 28.498 -15.407 2.075 1.00 39.14 | N |
| | ATC | M 2334 N LEU A 149 | 20.300 2000 | |

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С
                                                               1.00 37.49
                                                        2.168
                                      27.269 -14.634
                  CA
                      LEU A 149
            2336
                                                               1.00 38.02
                                                                                     С
    MOTA
                                                        1.699
                                      26.071 -15.476
                      LEU A 149
            2338
                  CB
                                                                                      С
                                                               1.00 45.01
    ATOM.
                                                        2.049
                                      24.571 -15.300
                      LEU A 149
            2341
                  CG
                                                                                      С
    MOTA
                                                               1.00 46.47
                                      23.843 -16.146
                                                        1.018
                  CD1 LEU A 149
            2343
                                                                                      С
    ATOM
                                                               1.00 46.97
                                      24.051 -15.748
                                                        3.449
                  CD2 LEU A 149
    MOTA
            2347
                                                                                      C
                                                               1.00 41.29
                                                        3.619
                                      27.073 -14.349
                       LEU A 149
   MOTA
            2351
                  С
10
                                                                1.00 43.07
                                                        4.445
                                      27.374 -15.200
                       LEU A 149
            2352
                  0
                                                                                      N
     MOTA
                                                                1.00 43.88
                                                        3.957
                                      26.597 -13.160
                       PHE A 150
                  N
            2353
     MOTA
                                                                                      C
                                                                1.00 37.90
                                                        5.313
                                      26.128 -12.896
                       PHE A 150.
            2355
                  CA
                                                                                      С
     MOTA
                                                                1.00 36.97
                                                         6.146
                                      27.151 -12.168
                       PHE A 150
                  CB
            2357
                                                                1.00 38.62
                                                                                      C
     MOTA
                                      27.514 -10.855
                                                         5.616
                       PHE A 150
                   CG
            2360
                                                                                      С
15
     MOTA
                                                                1.00 43.40
                                      28.508 -10.731
                                                        4.664
                  CD1 PHE A 150
     MOTA
            2361
                                                                1.00 36.52
                                                         4.157
                                      28.849 -9.516
                   CE1 PHE A 150
     MOTA
            2363
                                                                1.00 39.56
                                                         4.609
                                              -8.415
                                      28.202
                       PHE A 150
                   CZ
            2365
     MOTA
                                                                1.00 32.53
                                                         5.564
                                      27.220
                                              -8.530
                   CE2
                       PHE A 150
             2367
     ATOM
                                                                                      С
                                                                1.00 36.36
                                                         6.055
                                       26.885 -9.737
                       PHE A 150
             2369
                   CD2
                                                                                      C
20
     MOTA
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                                                         5.122
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                       PHE A 150
             2371
                   С
     MOTA
                                                                1.00 41.82
                                                                                      0
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                                                         4.054
                       PHE A 150
             2372
                   0
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     MOTA
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                                       23.980 -12.071
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                                                                                      C
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25
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                                                         8.190
                                       23.371 -10.749
                       SER A 151
             2383
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     MOTA
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                                                         7.214
                                               -9.260
                                       21.985
                       LEU A 152
             2384
                                                                                       С
     MOTA
                                                                 1.00 36.45
                                                         8.435
                                       21.755
                                               -8.448
                       LEU A 152
             2386
                   CA
30
     MOTA
                                                                 1.00 35.08
                                               -7.166
                                                         8.446
                                       22.588
                       LEU A 152
                   СВ
     ATOM
             2388
                                                                 1.00 29.92
                                                         8.489
                                       24.121
                                                -7.237
                        LEU A 152
                   CG.
             2391
      MOTA
                                                                 1.00 28.56
                                                         8.014
                                                -5.957
                                       24.769
                   CD1 LEU A 152
             2393
                                                                                       С
      MOTA
                                                                 1.00 30.11
                                                         9.812
                                               -7.467
                                        24.536
                       LEU A 152
             2397
                    CD2
                                                                                       С
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                                        20.305
                        LEU A 152
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              2401
                                                                                       . 0
 35
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                                                                 1.00 49.31
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                                                          7.756
                                        19.591
                        LEU A 152
              2402
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      MOTA
                                                                                       N
                                               -8.069
-7.609
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                                        19.877
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                    N
      MOTA
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                        GLN A 153
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                    CA
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                        GLN A 153
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                    CB
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                    CG
                                                                                       С
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                                                         12.109
                                                -9.519
                        GLN A 153
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                    CD
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                                                                                       0
                                                                 1.00 58.66
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                                                         13.231
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      MOTA
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                                                         11.663
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                    NE2 GLN A 153
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      ATOM
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                        GLN A 153
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                    С
      MOTA
                                                                                        0
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                                                 -7.157
                                        18.980
                        GLN A 153
              2419
                    0
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 45
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                                                 -5.384
                                        18.830
                        LEU A 154
              2420
                    N
                                                                                        С
      MOTA
                                                                1.00 42.93
                                                         12.397
                                                 -4.410
                        LEU A 154
                                        19.057
              2422
                    CA
                                                                                        С
      MOTA
                                                                 1.00 45.84
                                                 -3.221
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                                       19.826
                        LEU A 154
              2424
                    CB
       MOTA
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                    CG
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  50
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                    CD2 LEU A 154
              2433
       MOTA
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                                                                                        C
                                         17.700
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                         LEU A 154
                     Ċ
              2437
       MOTA
                                                                                        0
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                                         16.804
                         LEU A 154
              2438
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                                                                                        N
                                                 -3.646
                                         17.538
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              2439
                     N
                                                                                        С
       ATOM
                                                 -3.612 14.763 1.00 51.90
                         CYS A 155
                                         16.180
       ATOM
              2441
                     CA
                                                                                        C
  55
                                                                 1.00 51.86
                                                         15.662
                                                 -4.865
                         CYS A 155
                                         15.927
               2443
                     CB
       ATOM
                                                                                        S
                                                                  1.00 51.81
                                                         14.975
                                                 -6.528
                                         15.554
                         CYS A 155
                     SG
       MOTA
               2446
                                                                  1.00 57.62
                                                         15.642
                                         15.967
                                                 -2.390
                         CYS A 155
                     C
       MOTA
               2447
                                                         16.878
                                                                  1.00 63.11
                                                 -2.476
                                         16.114
                         CYS A 155
                     0
       MOTA
               2448
                                                         15.041 1.00 58.85
                                                 -1.257
                                         15.631
                         GLY A 156
               2449
                     N
  60
       MOTA
                                                 -0.072 15.830 1.00 62.65
                         GLY A 156
                                         15.380
               2451
                     CA
       MOTA
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| | | | | | | | | | | | _ |
|------------|--------------|--------------|-------|-------------|---|--------|---------|--------|------------|---|------------|
| 5 | MOTA | 2454 | С | GLY A 156 | | 14.226 | -0.446 | 16.728 | 1.00 66.48 | | C |
| • | | 2455 | 0 | GLY A 156 | | 13.447 | -1.309 | 16.342 | 1.00 69.64 | | 0 |
| | ATOM | 2456 | N | ALA A 157 | | 14.088 | 0.144 | 17.910 | 1.00 69.44 | | N |
| | ATOM | 2458 | CA | ALA A 157 | | 12.896 | -0.169 | 18.704 | 1.00 72.46 | | C |
| | ATOM | 2460 | CB | ALA A 157 | | 13.304 | -0.588 | 20.111 | 1.00 75.06 | | C |
| 10 | ATOM | 2464 | C | ALA A 157 | | 11.799 | 0.960 | 18.698 | 1.00 73.42 | | С |
| | ATOM | 2465 | 0 | ALA A 157 | | 10.749 | 0.888 | 19.359 | 1.00 73.68 | | 0 |
| | ATOM | 2466 | N | GLY A 158 | | 12.015 | 2.000 | 17.926 | 1.00 74.47 | | N |
| | ATOM | 2468 | CA | GLY A 158 | | 11.010 | 3.043 | 17.837 | 1.00 78.58 | | С |
| | ATOM. | 2471 | C | GLY A 158 | | 10.829 | 3.954 | 19.059 | 1.00 82.73 | | С |
| 15 · | ATOM | 2472 | ō | GLY A 158 | | 9.947 | 4.825 | 19.033 | 1.00 85.96 | | 0 |
| 15 | ATOM | 2473 | N | PHE A 159 | | 11.633 | 3.774 | 20.115 | 1.00 83.55 | | N |
| | ATOM | 2475 | CA | PHE A 159 | | 11.564 | 4.626 | 21.313 | 1.00 85.05 | | С |
| | MOTA | 2477 | CB | PHE A 159 | | 10.558 | 4.054 | 22.277 | 1.00 85.74 | | С |
| • | ATOM | 2480 | CG | PHE A 159 | | 10.993 | 2.748 | 22.855 | 1.00 82.94 | | C . |
| 20 | ATOM | 2481 | | PHE A 159 | | 10.305 | 1.593 | 22.561 | 1.00 82.82 | | С |
| 20 | ATOM | 2483 | | PHE A 159 | | 10.717 | 0.373 | 23.096 | 1.00 83.66 | | С |
| | MOTA | 2485 | CZ | PHE A 159 | | 11.831 | 0.325 | 23.935 | 1.00 82.59 | | С |
| | ATOM | 2487 | | PHE A 159 | | 12.519 | 1.491 | 24.228 | 1.00 80.31 | | · C |
| | ATOM | 2489 | | PHE A 159 | | 12.099 | 2.683 | 23.686 | 1.00 79.87 | | С |
| 25 | ATOM | 2491 | | PHE A 159 | | 12.910 | 4.671 | 22.044 | 1.00 87.61 | | С |
| 23 | ATOM | 2492 | o | PHE A 159 | | 13.494 | 3.624 | 22.302 | 1.00 87.56 | | 0 |
| | ATOM | 2493 | N | PRO A 160 | | 13.383 | 5.862 | 22.418 | 1.00 89.61 | | N |
| | MOTA | 2494 | CA | PRO A 160 | | 14.743 | | 22.954 | 1.00 91.86 | | С |
| • | ATOM | 2496 | СВ | PRO A 160 | | 14.714 | 7.423 | 23.610 | 1.00 92.67 | | C |
| 30 | ATOM | 2499 | CG | PRO A 160 | | | 8.102 | 23.127 | 1.00 90.33 | | C |
| 50 | ATOM | 2502 | CD | PRO A 160 | | 12.656 | 7.139 | 22.372 | 1.00 90.15 | | С |
| | ATOM | 2505 | C | PRO A 160 | | 15.261 | 5.019 | 23.970 | 1.00 91.59 | | С |
| • | ATOM | 2506 | ŏ | PRO A 160 | | 14.535 | 4.311 | 24.654 | 1.00 87.47 | | 0 |
| | ATOM | 2507 | N . | LEU A 161 | | 16.582 | 5.002 | 24.046 | 1.00 94.49 | | N |
| 35 | ATOM | 2509 | CA | LEU A 161 | | 17.318 | 4.103 | 24.906 | 1.00 97.03 | | С |
| 33 | ATOM | 2511 | CB | LEU A 161 | | 17.885 | 2.918 | 24.078 | 1.00 96.28 | | С |
| | ATOM | 2514 | CG | LEU A 161 | | 17.017 | 1.707 | 23.671 | 1.00 94.82 | | С |
| | ATOM | 2516 | | LEU A 161 | | 17.658 | 0.923 | 22.493 | 1.00 93.82 | | С |
| | ATOM | 2520 | | LEU A 161 | | 16.735 | 0.783 | 24.864 | 1.00 93.08 | | С |
| 40 | MOTA | 2524 | C | LEU A 161 | | 18.475 | 4.906 | 25.503 | 1.00 98.82 | | С |
| -10 | ATOM | 2525 | ō | LEU A 161 | | 18.848 | 5.967 | 24.987 | 1.00 98.25 | | 0 |
| | ATOM | 2526 | N | GLN A 162 | | 19.013 | 4.404 | 26.608 | 1.00101.00 | | N |
| | ATOM | 2528 | CA | GLN A 162 | | 20.290 | 4.865 | 27.135 | 1.00101.95 | | С |
| | ATOM | 2530 | | GLN A 162 | | 20.225 | 5.088 | 28.660 | 1.00103.13 | | С |
| 45 | ATOM | 2533 | CG | GLN A 162 | | 19.060 | 5.934 | 29.201 | 1.00102.96 | | С |
| -1.5 | ATOM | 2536 | CD | GLN A 162 | | 18.651 | . 5.522 | 30.624 | 1.00104.66 | | С |
| | ATOM | 2537 | | L GLN A 162 | | 17.703 | 6.076 | 31.190 | 1.00104.03 | | 0 |
| · : | ATOM | 2538 | | 2 GLN A 162 | | 19.365 | | 31.196 | 1:00103.68 | | N |
| | ATOM | 2541 | C | GLN A 162 | | 21.315 | 3.748 | 26.850 | 1.00102.26 | | С |
| 50 | ATOM | 2542 | 0. | GLN A 162 | | 20.958 | 2.612 | 26.522 | | | 0 |
| 50 | ATOM | 2543 | N. | GLN A 163 | | 22.593 | | 26.965 | 1.00104.53 | | N |
| | | 2545 | CA | GLN A 163 | | 23.655 | 3.073 | 26.995 | 1.00105.21 | • | С |
| | MOTA | 2547 | | GLN A 163 | | 24.906 | 3.716 | | 1.00105.72 | | C |
| | ATOM ATOM | 2550 | CG | GLN A 163 | | 26.028 | 2.741 | 27.928 | 1.00105.46 | | C |
| 55 | | 2553 | | GLN A 163 | | 27.384 | 3.435 | 27.930 | 1.00103.07 | | C |
| JJ | ATOM | | | 1 GLN A 163 | | 27.767 | 4.048 | 28.924 | 1.00 96.11 | | Ó. |
| • 1 | MOTA | 2554 | | 2 GLN A 163 | | 28.105 | | 26.814 | 1.00101.46 | | N |
| | ATOM | 2555 2558 | C NE. | GLN A 163 | • | 23.314 | | 27.894 | 1.00105.84 | | С |
| | MOTA | | | GLN A 163 | | 23.625 | | | 1.00105.65 | | 0 |
| <i>6</i> 0 | MOTA | 2559 | | SER A 164 | | 22.684 | | | | | N |
| 60 | ATOM | 2560 | | | | 22.315 | | | | | С |
| | ATOM | 2562 | CA | SEV W TO4 | | | 7.270 | | | | |

| 5 10 | MOTA MOTA MOTA MOTA MOTA MOTA | 2564 2567 2569 2570 2571 | CB OG C O | SER A | A 164 A 164 A 164 | | 21.632 21.798 21.335 | 1.798 1.017 0.192 | 31.227 32.400 29.374 | 1.00106.94 1.00107.14 1.00105.64 | | - | | C . |
|---------|--------------------------------------|--------------------------------------|--------------------|-------|-------------------------|---|----------------------------|-------------------------|----------------------------|--|---|----|---|-----|
| | ATOM ATOM ATOM ATOM ATOM | 2567 2569 2570 | OG C | SER A | A 164 A 164 | | | | | | | - | | |
| 10 | ATOM ATOM ATOM ATOM | 2569 2570 | С | SER 2 | A 164 | • | | 0 192 | 29.374 | 1.00105.64 | | - | | С |
| 10 | ATOM ATOM ATOM | 2570 | | | | | | | | | | | | |
| 10 | ATOM ATOM | | U | | A 16/ | | 21.407 | -1.065 | 29.492 | 1.00105.75 | | | | 0 |
| 10 | ATOM | 25/1 | 1.1 | | A 164 | | 20.403 | 0.835 | 28.682 | 1.00102.30 | | | | N |
| 10 | | | N | | A 165 | | | 0.105 | 27.976 | 1.00 98.16 | | | | C |
| | | 2573 | CA | | A 165 | | 19.381 | | | 1.00 98.15 | | | | č |
| | MOTA | 2575 | CB | | A 165 | | 18.355 | 1.082 | 27.415 | | • | | | c |
| | MOTA | 2578 | CG | | A 165 | | 17.997 | 2.126 | 28.479 | 1.00 99.91 | | | | C |
| | ATOM | 2581 | CD | | A 165 | | 16.584 | 2.687 | 28.403 | 1.00 98.66 | | | | |
| | MOTA | 2582 | OE1 | GLU | A 165 | | 15.621 | 1.933 | 28.642 | 1.00 94.69 | | | | 0 |
| 15 | MOTA | 2583 | OE2 | GLU | A 165 | | 16.444 | 3.900 | 28.123 | 1.00100.25 | | | | 0 |
| | MOTA | 2584 | С | GLU . | A 165 | | 20.072 | -0.690 | 26.891 | 1.00 95.52 | | | | С |
| | ATOM | 2585 | 0 | GLU . | A 165 | | 19.903 | -1.909 | 26.807 | 1.00 92.32 | | | | . 0 |
| | ATOM | 2586 | N | | A 166 | | 20.884 | 0.002 | 26.095 | 1.00 92.23 | | | | N |
| | ATOM | 2588 | CA | | A 166 | | 21.552 | -0.618 | 24.959 | 1.00 90.08 | | | | С |
| 20 | ATOM | 2590 | СВ | | A 166 | | 22.637 | 0.280 | 24.385 | 1.00 89.46 | | | | С |
| 20 | | | | | A 166 | | 23.997 | -0.471 | 24.238 | 1.00 89.54 | | | | С |
| | MOTA | 2592 | | | | | 22.180 | 0.834 | 23.067 | 1.00 89.64 | | | | С |
| | ATOM | 2596 | | | A 166 | | • | | 25.275 | 1.00 89.54 | | | | č |
| | MOTA | 2600 | С | | A 166 | | 22.155 | -1.969 | | 1.00 90.45 | | | | ō |
| | ATOM | 2601 | 0 | | A 166 | : | 21.868 | -2.949 | 24.587 | | • | | | N |
| 25 | MOTA | 2602 | N | | A 167 | | 22.988 | -2.039 | 26.306 | 1.00 89.05 | | | | |
| | MOTA | 2604 | CA | LEU | A 167 | | 23.644 | -3.308 | 26.620 | 1.00 88.10 | | | | C |
| | ATOM | 2606 | CB | ΓΕŃ | A 167. | | 24.572 | -3.201 | 27.852 | 1.00 87.51 | | | | C |
| | ATOM | 2609 | СĠ | LEU | A 167 | - | 25.665 | -2.130 | 27.780 | 1.00 89.06 | • | | | С |
| | ATOM | 2611 | CD1 | LEU | A 167. | | 25.990 | -1.526 | 29.151 | 1.00 88.01 | | | | С |
| 30 | ATOM | 2615 | CD2 | LEU | A 167 | | 26.921 | -2.670 | 27.122 | 1.00 88.50 | | | | С |
| | ATOM | 2619 | С | LEU | A 167 | | 22.606 | -4.403 | 26.851 | 1.00 84.50 | | | | С |
| | ATOM | 2620 | Ō | | A 167 | | 22.770 | -5.521 | 26,386 | 1.00 82.46 | | | | 0 |
| | ATOM | 2621 | N. | | A 168 | | 21.533 | -4.071 | 27.554 | 1.00 82.79 | | | | N |
| - | ATOM | 2623 | CA | | A 168 | | 20.565 | -5.083 | 27.974 | 1.00 83.99 | | | | С |
| 25 | | | CB · | | A 168 | | 19.807 | -4.567 | | 1.00 84.06 | | | | С |
| 35 | ATOM | 2625 | | | | | 19.560 | -5.604 | 26.929 | 1.00 84.00 | | ٠ | | C |
| | ATOM | 2629 | C | | A 168 | | 18.918 | -6.627 | 27.179 | 1.00 83.07 | | | | ō |
| | ATOM | 2630 | 0 | | A 168 | | | | | 1.00 82.75 | | | | N |
| | ATOM | 2631 | N | | A 169 | | 19.423 | -4.940 | 25.776 | 1.00 82.75 | | | | C |
| 4.0 | ATOM | 2633 | CA | | A 169 | | 18.339 | -5.295 | 24.845 | | | | | |
| 40 | MOTA | 2635 | CB | | A 169 | | 17.199 | -4.258 | 24.968 | 1.00 83.85 | | | | Ċ |
| | ATOM | 2638 | OG | | A 169 | | 16.810 | -4.032 | 26.327 | 1.00 80.23 | | | • | 0 |
| | ATOM | 2640 | C | SER | A 169 | | 18.735 | -5.521 | 23.349 | 1.00 81.77 | | | | С |
| | MOTA | 2641 | 0 | SER | A 169 | | 19.377 | -4.675 | 22.718 | 1.00 80.20 | | | | 0 |
| | ATOM | 2642 | N | VAL | A 170 | | 18.303 | -6.674 | 22.816 | 1.00 79.25 | | | | N |
| 45 | ATOM | 2644 | CA | VAL | A 170 | | 18.634 | -7.170 | 21.469 | 1.00 74.78 | | | | С |
| | ATOM | 2646 | CB | VAL | A 170 | | 17.885 | -8.506 | 21.198 | 1.00 76.32 | • | | | C |
| | ATOM | 2648 | CG1 | | A 170 | | 18.278 | -9.111 | 19.831 | 1.00 75.02 | | | • | С |
| | ATOM | 2652 | | | A 170 | | 18.143 | -9.504 | 22.334 | 1.00 77.47 | | | | С |
| | ATOM | 2656 | C | | A 170 | | 18.329 | -6.185 | 20.326 | 1.00 70.08 | | | | С |
| 50 | | 2657 | ŏ | | A 170 | | 17.197 | -5.720 | 20.160 | 1.00 70.47 | | | | 0 |
| JU, | ATOM | | | | | | 19.345 | -5.895 | 19.525 | 1.00 58.93 | | | | N |
| | MOTA | 2658 | N | | A 171 | | | | 18.482 | 1.00 51.34 | | | | c |
| | MOTA | 2660 | CA | | A 171 | | 19.208 | -4.921 | | | | | | č |
| | ATOM | 2663 | C | | A 171 | | 19.305 | -5.525 | 17.115 | 1.00 47.82 | | | | |
| | MOTA | 2664 | 0 | | A 171 | | 19.166 | -4.812 | 16.149 | | | | | 0 |
| 55 | MOTA | 2665 | N | GLY | A 172 | | 19.548 | -6.821 | 16.992 | 1.00 43.16 | • | | | N |
| | MOTA | 2667 | CA | | A 172 | | 19.604 | -7. _, 381 | 15.654 | 1.00 40.82 | | | : | C |
| | ATOM | 2670 | С | GLY | A 172 | | 20.369 | -8.678 | 15.473 | 1.00 42.31 | | | | С |
| | ATOM | 2671 | 0 | | A 172 | | 20.653 | -9.404 | 16.439 | 1.00 39.19 | | | | 0 |
| | MOTA | 2672 | N | | A 173 | • | 20.705 | -8.960 | 14.214 | 1.00 39.65 | | | | N |
| 60 | ATOM | 2674 | CA | | A 173 | | | -10.233 | 13.857 | 1.00 37.97 | | | • | C |
| 50 | ATOM | 2676 | CB | | A 173 | | | -11.203 | 13.497 | 1.00 36.33 | | | | С |
| | MIUH | 20,0 | J | ODI | | | | | | , = = 1.33 | | ٠. | | |

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19.416 -11.435 14.634
                                                                1.00 46.54
                       SER A 173
             2679
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                                                                                       С
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                                       22.205 -10.181
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                       SER A 173
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                                       21.805 -9.673
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                       SER A 173
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                       MET A 174
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                                                                                       C
                       MET A 174
                                                        11.516
     MOTA
             2698
                   С
                                                                                       O
                       MET A 174
                                       25.013 -13.111
                                                        12.356
                                                                 1.00 48.31
15
     ATOM
             2699
                   0
                                                                 1.00 38.41
                                                                                       N
                       ILE A 175
                                       24.003 -12.875
                                                        10.383
             2700
     MOTA
                   N
                                                                                       C
                                                                 1.00 37.39
                                       23.939 -14.288
                                                        10.136
                       ILE A 175
     ATOM
             2702
                   CA
                                                                 1.00 39.69
                                                                                       С
                       ILE A 175
                                       22.628 -14.676
                                                         9.443
             2704
                   CB
     MOTA
                                                                 1.00 40.97
                                       21.448 -14.387
                                                        10.364
             2706
                   CG1 ILE A 175
     MOTA
                                                                 1.00 36.79
                                                        11.578
                                       21.449 -15.213
             2709
                   CD1 ILE A 175
20
     ATOM
                                                                 1.00 35.35
                                                                                       C
                                       22.653 -16.089
                                                         9.035
                   CG2 ILE A 175
     MOTA
             2713
                                                                                       С
                       ILE A 175
                                       25.021 -14.522
                                                         9.202
                                                                 1.00 38.73
     ATOM
             2717
                   С
                                                                 1.00 40.30
                                                                                       0
                                                         8.037
                   0
                       ILE A 175
                                       24.892 -14.246
             2718
     ATOM
                                                                 1.00 42.09
                                                                                       N
                                       26.109 -15.038
                                                         9.722
                       ILE A 176
             2719
                   N
     ATOM
                                                                 1.00 37.74
                                                                                       C
                       ILE A 176
                                                         8.926
25
             2721
                   CA
                                       27.257 -15.301
     ATOM
                                                                                       С
                                                                 1.00 35.36
                                       28.382 -15.377
                                                         9.844
             2723
                   CB
                       ILE A 176
     MOTA
                                       28.371 -14.125
                                                        10.699
                                                                 1.00 32.86
                   CG1
                       ILE A 176
     MOTA
             2725
                                                                                       С
                                                                 1.00 37.77
                                       29.740 -13.602
                                                        11.051
                       ILE A 176
     ATOM
             2728
                   CD1
                                                                                       C
                                       29.673 -15.621
                                                         9.060
                                                                 1.00 38.65
                   CG2 ILE A 176
     ATOM
             2732
                                                                                       С
                                                                 1.00 43.85
30
                                                         8.202
                       ILE A 176
                                       27.119 -16.617
             2736
                   С
     ATOM .
                                                                                       0
                                                                 1.00 49.67
                                       27.178 -17.681
                                                         8.802
                       ILE A 176
     MOTA
             2737
                   0
                                                                 1.00 44.93
                                                                                       N
                                                         6.912
             2738
                   N
                       GLY A 177
                                       26.890 -16.568
     MOTA
                                                         6,139
                                                                                       C
                                                                 1.00 45.46
                                       27.003 -17.783
             2740
                       GLY A 177
     ATOM .
                   CA
                                                                 1.00 42.70
                                                                                       С
                                                         5.673
                                       25.734 -18.428
             2743
                   С
                       GLY A 177
     ATOM
                                                          5.054
                                                                 1.00 47.24
                                                                                       Ŏ
                       GLY A 177
                                       25.751 -19.498
35
             2744
     MOTA
                   0
                                                                 1.00 40.94
                                                                                       N
                       GLY A 178
                                       24.619 -17.791
                                                          5.934
             2745
                   N
     MOTA
                                                                 1.00 38.84
                                                                                       C
                       GLY A 178
                                       23.369 -18.400
                                                          5.553
     MOTA
             2747
                   CA
                                                                 1.00 36.04
                                       22.355 -17.317
                                                          5.705
     MOTA
             2750
                   С
                       GLY A 178
                                                          6.066
                                       22.754 -16.229
                                                                 1.00 32.65
      MOTA
             2751
                   0
                        GLY A 178
                                                                 1.00 38.29
                                                                                        N
                                       21.086 -17.636
                                                          5.418
40
                        ILE A 179
      MOTA
             2752
                   N
                                       19.922 -16.748
                                                          5.502
                                                                 1.00 36.73
                       ILE A 179
      MOTA
             2754
                   CA
                                       19.262 -16.733
                                                          4.137
                                                                 1.00 38.18
                        ILE A 179
             2756
                   CB
      MOTA
                                                                                        С
                                                                 1.00 38.79
                   CG1 ILE A 179
                                       20.269 -16.324
                                                          3.069
             2758
      MOTA
                                                                 1.00 37.73
                                                                                        С
                                                          1.644
                   CD1 ILE A 179
                                        19.789 -16.538
      MOTA
             2761
                                                          4.105
                                                                 1.00 40.58
                                        18.144 -15.825
 45
      ATOM
             2765
                   CG2 ILE A 179
                                                                 1.00 39.59
                                        19.019 -17.446
                                                          6.489
                        ILE A 179
             2769
                   С
      MOTA
                                                                 1.00 42.86
                                                                                        0
                                       18.914 -18.666
                                                          6.450
                        ILE A 179
      ATOM
             2770
                   0
                                                                  1.00 43.92
                                                                                        N
                                                          7.387
                        ASP A 180
                                        18.355 -16.727
      MOTA
             2771
                   N
                                        17.497 -17.405
                                                          8.388
                                                                  1.00 40.32
                        ASP A 180
             2773
                   CA
      MOTA
                                                                  1.00 42.54
 50
                   CB
                        ASP A 180
                                        17.913 -17.030
                                                          9.788
      MOTA.
             2775
                                                                  1.00 45.20
                                                                                        С
                                                         10.824
      ATOM ·
             2778
                   CG
                        ASP A 180
                                        16.967 -17.607
                                                                  1.00 38.88
                                                                                        0
                                        17.452 -17.999
15.717 -17.695
                                                         11.899
      ATOM'
             2779
                   OD1 ASP A 180
                                                                                        0
                                                         10.630
                                                                  1.00 43.52
                   OD2 ASP A 180
      MOTA
             2780
                                                                 1.00 38.18
                                        16.012 -17.138
                                                          8.278
             2781
                   C.
                        ASP A 180
      ATOM
                                        15.533 -16.094
                                                                  1.00 44.65
                                                                                        0
                                                          8.669
                        ASP A 180
 55
             2782
                   0.
      ATOM
                                        15.272 -18.105
                                                          7.782
                                                                  1.00 42.63
                                                                                        N
                        HIS A 181
      ATOM
             2783
                   N
                        HIS A 181
                                       13.864 -17.928
                                                          7.490
                                                                  1.00 41.71
                                                                                        С
             2785
                   CA
      MOTA
                                                                                        C
                                                          6.973
                                                                  1.00 48.30
             2787
                    CB
                        HIS A 181
                                       13.320 -19.226
      MOTA
                                                                                        C
                        HIS A 181
                                       13.911 -19.569
                                                         . 5.657
                                                                  1.00 63.31
      MOTA
             2790
                    CG
                                       13.525 -18.933
                                                          4.495
                                                                  1.00 74.50
                    ND1 HIS A 181
 60
             2791
      MOTA
                                        14.230 -19.409
                                                          3.483
                                                                  1.00 79.36
             2793
                    CE1 HIS A 181
      ATOM .
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| · 5 | MOTA | 2795 | NE2 | HIS A | 181 | ٠ | 15.065 | -20.328 | 3.950 | 1,00 79.2 | 7 | | N |
|------|-------|--------|------------|--------|-----|---|--------|---------|--------|------------|----------|-----|-----|
| | ATOM- | 2797 | CD2 | HIS A | 181 | | 14.890 | -20.439 | 5.310 | 1.00 71.5 | 5 | | С |
| | ATOM | 2799 | С | HIS A | | | | -17.340 | 8.538 | 1.00 37.1 | | | Ċ |
| | | | Ö | HIS A | | | | | | | | | |
| | ATOM | 2800 | | | | | | -16.873 | 8.232 | 1.00 39.5 | | | 0 |
| | ATOM | 2801 | N | SER A | | | | -17.329 | 9.773 | 1.00 37.6 | | | N |
| 10 | MOTA | 2803 | CA | SER A | 182 | | 12.603 | -16.703 | 10.793 | 1.00 41.5 | L | | С |
| | ATOM | 2805 | CB | SER A | 182 | | 12.986 | -17.234 | 12.149 | 1.00 42.1 | 7 | | С |
| | ATOM | 2808 | OG | SER A | | | | -16.913 | 12.339 | 1.00 43.8 | | | 0 |
| | ATOM | 2810 | C · | SER A | | | | -15.204 | 10.848 | 1.00 39.2 | | | Ċ |
| | ATOM | | ō | SER A | | | | | | 1.00 46.7 | | | |
| 15 | | | | | | | | -14.548 | 11.554 | | | | 0 |
| 13 | MOTA | 2812 | | LEU A | | | | -14.644 | 10.130 | 1.00 38.9 | | | N |
| | ATOM | 2814 | | LEU A | | | | -13.201 | 10.197 | 1.00 35.6 | | | С |
| | ATOM | 2816 | . CB | LEU A | | | 15.456 | -12.924 | 10.189 | 1.00 33.3 | 3 | | C |
| | ATOM | 2819 | CG | LEU F | 183 | | 16.258 | -13.474 | 11.374 | 1.00 31.83 | 3 | | C |
| • | ATOM | 2821 | CD1 | LEU A | 183 | | 17.709 | -13.477 | 11.088 | 1.00 31.7 | 5 | | С |
| 20 | ATOM | 2825 | CD2 | LEU A | 183 | | | -12.666 | 12.607 | 1.00 41.8 | | | C |
| | ATOM | 2829 | С | LEU P | | | | -12.400 | 9.068 | 1.00 38.0 | | • | Č |
| | ATOM | 2830 | ō | | | | | | | | | | |
| | | | | LEU A | | | | -11.288 | 8.820 | 1.00 42.0 | | | 0 |
| | MOTA | 2831 | N | TYR A | | | | -12.956 | 8.367 | 1.00 44.4 | | | N |
| | ATOM | 2833 | CA | TYR P | | | | -12.209 | 7.320 | 1.00 33.3 | 1 | | C |
| 25 | MOTA | . 2835 | CB | TYR A | 184 | | 12.516 | -12,087 | 6.063 | 1.00 38.73 | 2 | | С |
| | ATOM | 2838 | CG | TYR P | 184 | | 12.775 | -13.281 | 5.134 | 1.00 35.8 | 6 | | С |
| | ATOM | 2839 | CD1 | TYR A | 184 | | | -14.047 | 5.248 | 1.00 43.79 | 9 | | Ċ |
| | ATOM | 2841 | | TYR A | | | • | -15.099 | 4.406 | 1.00 39.7 | | | Ċ |
| • | MOTA | 2843 | CZ | TYR A | • | | | -15.400 | 3.426 | 1.00 40.9 | | | .c |
| 30 | ATOM | 2844 | OH | TYR A | | | | | | | | | |
| 50 | | | | | | | | -16.460 | 2.577 | 1.00 45.5 | | • | 0 |
| | ATOM | 2846 | | TYR A | | | • | -14.656 | 3.277 | 1.00 38.7 | | | С |
| | ATOM | 2848 | | TYR A | | | | -13.599 | 4.127 | 1.00 36.4 | 7 | | C. |
| | ATOM | 2850 | C. | TYR A | 184 | | | -12.811 | 7.005 | 1.00 36.10 | 5 | | С |
| | MOTA | 2851 | ,0 | TYR A | 184 | | 10.067 | -13.961 | 7.352 | 1.00 30.8 | 3 | | 0 |
| 35 | ATOM | 2852 | N | THR A | 185 | | | -12.023 | 6.383 | 1.00 37.93 | 3 | | N |
| | ATOM | 2854 | CA | THR A | | | | -12.549 | 5.846 | 1.00 40.8 | | | C |
| | ATOM | 2856 | CB | THR A | | | | -11.913 | 6.441 | 1.00 43.1 | | | Ċ |
| | ATOM | 2858 | | THR A | | | | -10.491 | 6.207 | 1.00 43.9 | | | Ö |
| | ATOM | 2860 | | | | | | | | | | | |
| 40 | | | | THR A | | | | -12.140 | 7.970 | 1.00 42.48 | | | C |
| 40 | MOTA | 2864 | С | THR A | | | | -12.271 | 4.378 | 1.00 37.63 | | | С |
| | MOTA | 2865 | 0 | THR A | | | | -11.408 | 3.929 | 1.00 36.3 | 7 | | O. |
| | ATOM | 2866 | N | GLY A | 186 | | 7.321 | -12.992 | 3.637 | 1.00 34.8 | 5 | | N |
| | ATOM | 2868 | CA | GLY A | 186 | | 7.221 | -12.791 | 2.205 | 1.00 37.13 | <u>l</u> | | С |
| | ATOM | 2871 | С | GLY A | 186 | | 8.449 | ~13.300 | 1.469 | 1.00 38.69 |) | | С |
| 45 | ATOM | 2872 | 0 | GLY A | 186 | • | | -14.161 | 1.954 | 1.00 44.0 | | | Ō |
| | ATOM | 2873 | N | SER A | | | | -12.736 | 0.288 | 1.00 41.4 | | | N |
| | ATOM | 2875 | CA | SER A | | | | -13.062 | -0.552 | • | | | |
| • | | | | | | | | | | 1.00 43.1 | | | C |
| | ATOM | 2877 | | | | | | -13.063 | | | | | Ċ |
| co . | ATOM | 2880 | OG | SER A | | | | -13.936 | -2.139 | 1.00 54.9 | | | 0 |
| 50 | ATOM | 2882 | С | SER A | | | | -12.059 | -0.443 | 1.00 44.8 | 1 | | С |
| | MOTA | 2883 | <u>O</u> | SER A | 187 | | 10.749 | -10.938 | 0.064 | 1.00 42.30 |) | | 0 |
| | MOTA | 2884 | N | LEU A | 188 | | 12.094 | -12.514 | -0.943 | 1.00 39.20 | | * . | N |
| | MOTA | 2886 | CA | LEU A | | | | -11.810 | -1.031 | 1.00 33.6 | | | C |
| | ATOM | 2888 | СВ | LEU A | | | | -12.824 | -0.789 | 1.00 28.6 | | | . C |
| 55 | ATOM | 2891 | CG | LEU A | | | | | | | | | |
| 55 | | | | | | | | -12.884 | 0.614 | 1.00 36.43 | | | C |
| | ATOM | 2893 | | LEU A | | | | -14.211 | 0.813 | 1.00 40.8 | | | . C |
| | ATOM | 2897 | | LEU A | | | | -11.777 | 0.889 | 1.00 34.4 | | | . C |
| | ATOM | 2901 | С | LEO. A | | | | -11.417 | -2.474 | 1.00 31.5 | | | С |
| | ATOM | 2902 | 0 | LEU A | 188 | | 13.359 | -12.268 | -3.294 | 1.00 41.6 |) | | 0 |
| 60 | MOTA | 2903 | N . | TRP A | 189 | | 13.803 | -10.177 | -2.822 | 1.00 31.39 | | | N |
| | MOTA | 2905 | CA | TRP A | | | 14.040 | | -4.230 | 1.00 33.70 | | | C |
| | | | | | | | | _ , | | | - | | • |

| | | | | | 100 | 13.132 | -8.688 | -4.683 | 1.00 | 39.33 | | | С |
|------|------|-------|------|-------|-------|--------|----------|-----------|-------|---------|----|-------|-----|
| 5 | MOTA | 2907 | | TRP A | | - | -9.074 | -4.947 | 1.00 | 37.95 | | | С |
| • | MOTA | 2910 | | TRP A | | 11.729 | | -4.033 | 1.00 | 35 87 | | | С |
| | MOTA | 2911 | | TRP A | | 10.779 | -9.313 | | 1.00 | | | | N |
| | MOTA | 2913 | | TRP A | | 9.600 | -9.646 | -4.649 | 1.00 | | | | c |
| | MOTA | 2915 | | TRP A | | 9.790 | -9.626 | -6.001 | | | | | c |
| 10 | MOTA | 2916 | CD2 | TRP A | 189 | 11.125 | -9.267 | -6.224 | 1.00 | | | | c |
| 10 | ATOM | 2917 | CE3 | TRP A | 189 | 11.586 | -9.181 | -7.539 | | 35.10 | | | |
| | ATOM | 2919 | | TRP A | | 10.725 | -9.447 | -8.559 | | 43.54 | | | C |
| | ATOM | 2921 | | TRP A | | 9.384 | -9.805 | -8.305 | | 44.03 | | | С |
| | | 2923 | | TRP A | | 8.904 | -9.898 | -7.034 | | 40.92 | | | С |
| 1.5 | ATOM | | | TRP A | | 15.493 | -9.361 | -4.344 | | 34.18 | | | С |
| 15 | ATOM | 2925 | | TRP A | | 15.950 | -8.570 | -3.567 | 1.00 | 34.73 | | | Ο. |
| | ATOM | 2926 | | TYR A | | 16.217 | -9.852 | -5.317 | | 34.76 | | | N |
| | ATOM | 2927 | N | TIK A | 100 | 17.603 | -9.539 | -5.412 | | 36.58 | • | | С |
| | MOTA | 2929 | | TYR A | | | -10.800 | -5.769 | | 38.76 | | | C. |
| • | MOTA | 2931 | | TYR A | | | | -4.657 | | 40.52 | | | С |
| 20 | MOTA | 2934 | | TYR A | | | -11.826 | | | 43.16 | | | C |
| | MOTA | 2935 | | TYR A | | | -12.875 | -4.609 | | 43.91 | | | Ċ |
| | MOTA | 2937 | | TYR A | | | -13.817 | -3.580 | | | | | č |
| | MOTA | 2939 | | TYR A | | | -13.685 | -2.615 | | 42.77 | | | ŏ |
| | ATOM | 2940 | OH | TYR A | 190 | 18.608 | -14.594 | -1.566 | | 46.77 | | | |
| 25 | ATOM | 2942 | CE2 | TYR F | 190 | | -12.642 | -2.677 | | 35.63 | | | C |
| . 23 | ATOM | 2944 | | | | 19.327 | -11.742 | -3.668 | | 35.67· | • | | C |
| | ATOM | 2946 | C | TYR F | 190 | 17.886 | -8.451 | -6.430 | | 38.30 | | | C |
| | | 2947 | ŏ | TYR A | | 17.248 | -8.420 | -7.424 | | 34.41 | | | 0 |
| | ATOM | | N | THR A | | 18.850 | | -6.133 | | 41.18 | | | N |
| 20 | MOTA | 2948 | | THR A | | 19.299 | | -7.025 | 1.00 | 37.26 | | | С |
| 30 | MOTA | 2950 | CA | | | 19.056 | | -6.438 | 1.00 | 38.25 | | | С |
| | MOTA | 2952 | CB | THR A | | 19.283 | | -7.448 | | 41.41 | | | О |
| | ATOM | 2954 | 0G1 | THR A | | 20.057 | | -5.419 | | 31.07 | | | C |
| | ATOM | 2956 | CG2 | THR A | | 20.782 | | -7.200 | | 39.94 | | | C |
| | MOTA | 2960 | C | | A 191 | 21.489 | | -6.264 | | 41.73 | | | 0 |
| 35 | ATOM | 2961 | 0 | | A 191 | | | -8.395 | | 39.23 | • | | N |
| | ATOM | 2962 | N | | A 192 | 21.281 | | | | 39.19 | | | С |
| | MOTA | 2963 | CA | | A 192 | 22.679 | | -10.111 | | 41.47 | | | С |
| | MOTA | 2965 | CB | | A 192 | 22.824 | | -10.111 | | 36.70 | | | С |
| | MOTA | 2968 | CG | | A 192 | 21.484 | | | | 41.63 | | | C |
| 40 | MOTA | 2971 | CD | | A 192 | 20.603 | | | | 41.91 | | | C |
| | MOTA | 2974 | С | | A 192 | 23.568 | | | | 43.47 | | | ō |
| | ATOM | 2975 | 0 | PRO . | A 192 | 23.16 | | | | | | | N |
| | MOTA | 2976 | N | ILE | A 193 | 24.78 | | | | 46.52 | | | C |
| | MOTA | 2978 | CA | ILE | A 193 | 25.82 | | | | 42.19 | | | . Ċ |
| 45 | MOTA | 2980 | CB | ILE | A 193 | 26.76 | | | | 38.18 | | | Č |
| | MOTA | 2982 | CG1 | ILE | A 193 | 26.15 | | | - | 41.41 | | | c |
| | ATOM | 2985 | | ILE | A 193 | 27.03 | | | • | 45.77 | | | C |
| | ATOM | 2989 | | | A 193 | 27.96 | 1 -5.447 | -5.994 | | 42.22 | | | |
| | ATOM | 2993 | | | A 193 | 26.60 | 3 -5.049 | -8.313 | 1.00 | 44.50 | | | C |
| 50 | | 2994 | | | A 193 | 27.21 | | 8 -8.984 | | 44.15 | | • | 0 |
| 50 | ATOM | 2995 | | | A 194 | 26.59 | | | 1.00 | 44.93 | | | Ŋ |
| | ATOM | | | | A 194 | | 4 -3.288 | | | 47.47 | | • • • | Ċ |
| | ATOM | -2997 | | | | 26.90 | | 3 -10.032 | | 52.04 | | | C |
| | MOTA | 2999 | | | A 194 | | | -11.424 | | 54.84 | | • | Ċ |
| , | MOTA | 3002 | | | A 194 | | | 11.320 | | 51.97 | ٠. | | C |
| 5,5 | ATOM | 3005 | | | A 194 | 27.41 | | 5 -12.548 | | 0 49.01 | | | N |
| | MOTA | 3008 | | | A 194 | 27.32 | | | | 0 45.93 | | | C |
| | MOTA | 3010 |) CZ | | A 194 | | | 7 -12.600 | | 0 41.67 | | | N |
| | MOTA | 3011 | | | A 194 | | | 9 -11.509 | | | | • | N |
| | MOTA | 3014 | NH2 | 2 ARG | A 194 | 27.49 | | 8 -13.742 | | 0 51.03 | | | · C |
| 60 | | 3017 | 7 C | ARG | A 194 | 28.76 | | 9 -9.869 | | 0 53.38 | | | 0 |
| | ATOM | | | | A 194 | | 31 -3.74 | 7 -10.92 | 1 1.0 | 0 57.83 | | | U |
| | | | | | | | | | | | • | | |

| | | | | | | | | | | | | | | _ |
|-----|-------|--------------|-----|---------|------------|------|---|--------|--------|--------|-------------|---|---|-----|
| 5 | ATOM | 3019 | N | ARG | Α | 195 | | 29.433 | -3.341 | -8.723 | 1.00 49.23 | | | N |
| _ | ATOM | 3021 | CA | ARG | | | | 30.887 | -3.378 | -8.698 | 1.00 49.56 | | | С |
| | ATOM | 3023 | CB | ARG | | | • | 31.470 | -1.973 | -8.965 | 1.00 49.15 | | | С |
| | ATOM | 3026 | CG | ARG. | | | | 32.684 | -1.929 | -9.832 | 1.00 45.49 | | | Ç |
| | ATOM | 3029 | CD | ARG | | | | 33.888 | -1.211 | -9.229 | 1.00 54.35 | | • | Ċ |
| 10 | ATOM | 3032 | NE | ARG | | | | 33.658 | 0.142 | -8.774 | 1.00 52.34 | | 1 | N |
| 10 | ATOM | 3034 | CZ | ARG | | | | 34.625 | 0.982 | -8.430 | 1.00 58.59 | • | + | С |
| | ATOM | 3035 | | ARG | | | | 35.892 | 0.624 | -8.476 | 1.00 59.01 | | • | N |
| - | ATOM | 3038 | | ARG | | | | 34.335 | 2.210 | -8.029 | 1.00 62.23 | | | N |
| | ATOM | 3041 | C . | ARG | | | | 31.317 | -3.740 | -7.314 | 1.00 51.05 | | | C |
| 15 | | 3041 | o . | ARG | | | | 30.795 | -3.169 | -6.362 | 1.00 44.37 | | | 0 |
| 13 | MOTA | | N. | GLU | | | • | 32.281 | | -7.173 | 1.00 52.25 | | | N |
| | ATOM | 3043 | | GLU | | | • | 32.723 | -4.988 | -5.831 | 1.00 53.43 | | | С |
| | ATOM | 3045 | CA | GLU | | | | 33.192 | -6.461 | -5.735 | 1.00, 57.30 | | | С |
| : | MOTA | 3047 | CB. | GLU | | | | 32.048 | -7.476 | -5.923 | 1.00 59.93 | | | C |
| 20 | ATOM | 3050 | CG | | | | | 32.485 | -8.961 | -5.919 | 1.00 65.83 | | | C |
| 20 | MOTA | 3053 | CD | GLU | | | | 32.977 | -9.443 | -6.966 | 1.00 59.79 | | | ō |
| | ATOM | 3054 | | GLU | | | | | -9.670 | -4.885 | 1.00 64.02 | | | ō |
| | ATOM | 3055 | | GLU | | | | 32.327 | -3.977 | -5.341 | 1.00 47.93 | | | Č |
| | MOTA | 3056 | C | GLU | | | | 33.758 | • | -5.563 | 1.00 47.03 | | | ŏ |
| , | MOTA | 3057 | 0 | GLU | | | , | 34.933 | -4.143 | | 1.00 44.26 | | | N |
| 25 | MOTA | 3058 | N | TRP | | | | 33.274 | -2.911 | -4.694 | 1.00 39.52 | | | C |
| | MOTA | 3060 | CA | TRP | | | - | 34.115 | -1.929 | -4.021 | 1.00 35.32 | | | c |
| | MOTA | 3062 | | TRP | | | | 34.594 | -0.730 | -4.922 | | | | C |
| | ATOM | 3065 | CG | TRP | | | | 33.660 | 0.246 | -5.517 | 1.00 40.87 | | | c |
| | MOTA | 3066 | | TRP | | | | 32.438 | 0.002 | -5.994 | • | | | N |
| 30 | ATOM. | 3068 | | TRP | | | | 31.860 | 1.157 | -6.468 | 1.00 45.72 | | | С |
| | ATOM | 3070 | | TRP | | | | 32.731 | 2.186 | -6.302 | 1.00 42.13 | | | C |
| | MOTA | 3071 | | TRP | | | | 33.885 | 1.649 | -5.705 | 1.00 45.88 | | | C |
| | MOTA | 3072 | , | TRP | | | | 34.945 | 2.509 | -5.427 | 1.00 46.01 | | | Ċ |
| | MOTA | 3074 | | TRP | | | | 34.813 | 3.842 | -5.746 | 1.00 47.92 | | | 0 |
| 35 | MOTA | 3076 | | TRP | | | | 33.651 | 4.330 | -6.338 | 1.00 50.66 | | | C |
| | MOTA | 3078 | | ŢRP | | | | 32.600 | 3.515 | -6.626 | 1.00 43.28 | | | C |
| | MOTA | 3080 | С | TRP | | | | 33.334 | -1.576 | -2.764 | 1.00 38.50 | | | C |
| | ATOM | 3081 | 0 | TRP | Α | 197 | | 33.528 | -2.184 | -1.733 | 1.00 49.55 | | | 0 |
| | MOTA | 3082 | ·N | TYR | A | 198 | | 32.472 | -0.599 | -2.786 | 1.00 38.10 | | | N |
| 40 | ATOM | 3084 | CA | TYR | Α | 198 | | 31.466 | -0.531 | -1.734 | 1.00 37.22 | | | C |
| | MOTA | 3086 | CB | TYR | A | 198 | | 30.770 | 0.851 | -1.643 | 1.00 35.77 | | | C |
| | ATOM | 3089 | CG | TYR | A | 198 | | 31.675 | 2.028 | -1.405 | 1.00 36.02 | | | C |
| | ATOM | 3090 | | TYR | | | | 31.813 | 2.562 | -0.142 | 1.00 38.94 | | | C |
| | ATOM | 3092 | CE1 | TYR | Α | 198 | | 32.633 | 3.626 | 0.094 | 1.00 39.66 | • | | C |
| 45 | ATOM | 3094. | CZ | TYR | Α | 198 | | 33.343 | 4.193 | -0.948 | 1.00 44.31 | | | C |
| | ATOM | 3095 | OH | | | 198 | | 34.174 | 5.269 | -0.701 | 1.00 46.07 | | | 0 |
| | ATOM | 3097 | CE2 | TYR | A | 198 | | 33.225 | 3.681 | -2.233 | 1.00 44.86 | | • | С |
| | ATOM | 3099 | CD2 | TYR | . A | 198 | ٠ | 32.386 | 2.595 | -2.448 | 1.00 42.57 | | | C |
| | ATOM | 3101 | C | TYR | Α | 198 | | 30.433 | -1.521 | | 1.00 33.99 | | | С |
| 50 | ATOM | 3102 | 0 | | | 198. | | 30.574 | -2.022 | -3.287 | 1.00 30.84 | | | . 0 |
| 0.0 | ATOM | 3103 | N | | | 199 | | 29.405 | -1.802 | -1.418 | 1.00 38.45 | | | N |
| | ATOM. | 3105 | CA | | | 199 | • | 28.256 | -2.557 | -1.900 | 1.00 37.49 | • | | С |
| | ATOM | 3107 | СВ | | | 199 | | 27.490 | -3.208 | -0.728 | 1.00 36.73 | | | С |
| | ATOM | 3110 | CG | | | 199 | | 28.233 | -4.329 | -0.047 | 1.00 32.48 | | | С |
| 55 | ATOM | 3111 | | TYR | | | | 28.787 | | 1.205 | 1.00 33.92 | • | | С |
| 55 | ATOM | 3113 | | TYR | | | | 29.453 | -5.141 | 1.822 | 1.00 32.06 | | | C. |
| | | 3115 | CZ | | | 199 | | 29.573 | | | 1.00 32.26 | | | С |
| | ATOM | 3115 | OH | | | 199 | | 30.243 | -7.369 | | 1.00 34.61 | | | 0 |
| | ATOM | | | YYR | | | | 29.024 | -6.485 | | | | | С |
| 60 | ATOM | 3118 3120 | | | | 199 | | 28.372 | | - | 1.00 33.21 | | | C |
| ou | MOTA | | | | | 199 | • | 27.368 | | | 1.00 42.41 | | | Ç |
| | ATOM | 3122 | C | * * * * | | 400 | | 21.500 | 1.525 | | | | | 7 |

| 5 | ATOM | 3123 | 0 | TYR A | 199 | | 26.418 | -0.978 | -2.075 | 1.00 | 45.22 | | | . 0 |
|------|--------------|--------------|-----|-------|--------|---|--------|----------------|------------------|------|----------------|----|-----|--------|
| - | ATOM | 3124 | N | GLU F | | | 27.702 | -1.272 | -3.910 | 1.00 | 43.18 | | • | N |
| | ATOM | 3126 | CA | GLU F | | • | 27.054 | -0.284 | -4.777 | 1.00 | 43.16 | | | С |
| | ATOM | 3128 | СВ | GLU A | | | 28.089 | 0.193 | -5.809 | 1.00 | | | | C |
| | ATOM | 3131 | CG | GLU A | | | 27.626 | 1.383 | -6.660 | 1.00 | 52.95 | | | С |
| 10 · | | 3134 | CD | GLU A | 200 | | 28.337 | 1.543 | -7.977 | 1.00 | 51.92 | | | С |
| | MOTA | 3135 | OE1 | GLU F | 200 | | 29.496 | 1.164 | -8.085 | 1.00 | | | | 0 |
| | ATOM | 3136 | OE2 | GLU A | 200 | | 27.715 | 2.055 | -8.901 | 1.00 | | | | 0 |
| | ATOM | 3137 | С | GLU A | A 200 | | 25.857 | -0.816 | -5.577 | | 44.00 | | | С |
| | ATOM | 3138 | 0 | GLU A | A 200 | | 25.993 | -1.789 | -6.319 | 1.00 | | | | Ο, |
| 15 | MOTA | 3139 | N | VAL A | | | 24.691 | -0.193 | -5.481 | | 37.72 | | | N |
| | ATOM | 3141 | CA | VAL A | 201 | | 23.583 | -0.713 | -6.250 | 1.00 | | | . 1 | C |
| | ATOM | 3143 | CB | VAL A | | | 22.598 | -1.332 | -5.374 | 1.00 | | | | C |
| | ATOM | 3145 | | VAL A | | | 23.127 | -2.629 | -4.926 | 1.00 | | | | C |
| • | MOTA | 3149 | CG2 | VAL A | | | 22.411 | -0.506 | -4.261 | 1.00 | | | | C |
| 20 | MOTA | 3153 | С | VAL A | | | 22.911 | 0.371 | -7.006 | 1.00 | | | | С |
| | ATOM | 3154 | 0 | VAL A | | | 23.235 | 1.474 | -6.781 | | 46.66 | | | 0 |
| - | ATOM | 3155 | N | | 1 202 | | 21.975 | 0.073 | -7.877 | | 41.86 | | | N |
| | ATOM | 3157 | CA | | 1 202 | • | 21.271 | 1.122 | -8.619 | | 45.62 | | | C |
| | MOTA | 3159 | СВ | | 1 202 | | 21.435 | 0.898 | -9.997 | | 47.37 | | | C |
| 25 | MOTA | 3161 | | ILE A | | | 22.924 | | -10.223 | | 50.21 | | • | C |
| ٠. | MOTA | 3164 | | ILE A | | | 23.240 | | -11.515 | | 50.75 | | | C |
| | ATOM | 3168 | | | 1 202. | | 20.619 | | -10.700 | | 47.14 46.10 | | | C C |
| | ATOM | 3172 | C | | A 202 | | 19.779 | 1.335 | -8.517 | | | | | 0 |
| 20 | ATOM | 3173 | 0 | | A 202 | | 19.001 | 0.401 | -8.788 | | 46.34 | | | N |
| 30 | ATOM | 3174 | N | | A 203 | | 19.438 | 2.595 | -8.195 | | 44.21 41.01 | | | C |
| | ATOM | 3176 | CA | | A. 203 | | 18.092 | 3.089 | -7.882 | | 42.75 | | | c |
| | ATOM | 3178 | CB | | A 203 | • | 18.195 | 4.290 | -6.931 -5.629 | | 36.25 | ٠. | | c |
| | ATOM | 3180 | | ILE A | | | 18.885 | 3.856 4.666 | -3.629 | | 37.62 | | | C |
| 35 | ATOM | 3183 3187 | | ILE A | | | 16.754 | 4.972 | -6.754 | * | 42.00 | | | c |
| 33 | MOTA MOTA | 3191 | CGZ | | A 203 | , | 17.508 | 3.646 | -9.096 | | 43.71 | • | | Ċ |
| | ATOM | 3192 | Ö | | A 203 | | 18.164 | 4.384 | -9.797 | | 45.90 | | | ō |
| | ATOM | 3193 | N | | A 204 | | 16.259 | 3.369 | -9.374 | | 43.96 | • | | N |
| | ATOM | 3195 | | | A 204 | | 15.807 | | -10.662 | | 43.46 | | | С |
| 40 | ATOM | 3197 | CB | | A 204 | | 15.743 | | -11.563 | | 47.55 | | | С |
| | ATOM | 3199 | | VAL | | | 17.031 | | -11.395 | 1.00 | 51.23 | | | C |
| | ATOM | 3203 | | VAL 2 | | | 14.676 | | -11.133 | 1.00 | 52.39 | | | Ċ |
| | MOTA | 3207 | · C | | A 204 | | 14.525 | 4.610 | -10.624 | 1.00 | 42.03 | | | С |
| | ATOM | 3208 | 0 | VAL 2 | A 204 | | 14.075 | 5.093 | -11.639 | 1.00 | 46.48 | | | 0 |
| 45 | ATOM | 3209 | N | ARG 2 | A 205 | | 13.944 | 4.739 | 9.445 | 1.00 | 40.50 | | | N |
| | MOTEA | 3211 | CA. | ARG 2 | A 205 | | 12.755 | 5.532 | -9.254 | 1.00 | 41.19 | | - | C |
| | MOTA | 3213 | CB | ARG 2 | A 205 | | 11.567 | 4.685 | -9.609 | 1.00 | 44.75 | | | С |
| | MOTA | 3216 | CG | ARG . | A 205 | | 10.235 | 5.385 | -9.532 | 1.00 | 49.25 | | | С |
| | MOTA | 3219 | CD | ARG . | A 205 | | 9.191 | 4.670 | -10.422 | 1.00 | 55.42 | | • | С |
| 50 | MOTA | 3222 | NE | ARG . | A 205 | | 7.775 | 4.754 | -10.007 | 1.00 | 57.55 | | | N |
| | ATOM | 3224 | CZ | ARG . | A 205 | : | 6.805 | | -10.797 | 1.00 | 56.49 | | | С |
| | ATOM | 3225 | NH1 | ARG . | A 205 | | 7.092 | 5.604 | -12.017 | | 54.80 | | | N |
| | MOTA | 3228 | NH2 | ARG . | A 205 | | 5.550 | | -10.377 | | 61.53 | | | N |
| | MOTA | 3231 | С | ARG . | A 205 | | 12.674 | 5.953 | -7.799 | | 38.57 | | | C |
| 55 | MOTA | 3232 | 0 | | A 205 | | 13.264 | 5.307 | -7.003 | | 40.72 | | | 0 |
| | ATOM | 3233 | N | | A 206 | | 11.961 | 7.032 | -7.462 | | 39.00 | | | N |
| .7 | | 3235 | CA | | A 206 | | 11.709 | 7.408 | -6.072 | | 35.25 | | | C |
| | ATOM | 3237 | CB | | A 206 | | 12.689 | 8.391 | | | 38.80 | | | ·C |
| | MOTA | 3239 | | | A 206 | | 12.331 | 8.891 | | | 40.25 | | | C |
| 60 | ATOM | 3243 | | | A 206 | | 14.073 | 7.800 | | | 45.84 | | | C |
| | MOTA | 3247 | С | VAL | A 206 | | 10.285 | 8.022 | -5.864 | 1.00 | 41.79 | | | С |

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-6.540
                                                                1.00 41.15
                      VAL A 206
                                       9.881
                                                9.004
     MOTA
            3248
                                                                1.00 43.20
                      GLU A 207
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                                                                1.00 39.16
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                                       8.124
                      GLU A 207
            3251
                  CA
     ATOM
                                                                                      C
                                                6.726
                                                       -4.872
                                                                1.00 41.81
                      GLU A 207
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            3253
                  CB
     ATOM
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                                                       -6.293
                      GLU A 207
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                                                6.501
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                  CG
     ATOM
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                                                                1.00 41.92
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    ATOM
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                      GLU A 207
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                                                       -3.150
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                      ILE A 208
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15
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                                                                                      С
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                                                       -1.819
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     MOTA
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                                                       -1.692
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            3268
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                      ILE A 208
     MOTA.
                                                                                      С
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                                                                1.00 42.36
                                               11.379
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                  CG1 ILE A 208
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            3270
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                                                                1.00 45.04
                  CD1 ILE A 208
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      MOTA
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| _ | | | | | | 0 100 | 13.673 -11.542 | 1.00 58.84 | | С |
|------|--------|-------|-----|-------------|---|--------|----------------|------------|---|-----|
| 5 | MOTA | 3356 | CB | LYS A 214 | | 9.120 | | 1.00 63.68 | | Č. |
| | ATOM | 3359 | CG | LYS A 214 | | 8.713 | 13.941 -12.984 | 1.00 65.33 | • | č |
| | MOTA | 3362 | CD | LYS A 214 | | 7.904 | 12.796 -13.625 | 1.00 65.28 | | č |
| | ATOM | 3365 | CE | LYS A 214 | | 8.338 | 12.533 -15.096 | 1.00 65.26 | | N |
| | MOTA | 3368 | NZ | LYS A 214 | | 7.187 | 12.419 -16.076 | 1.00 54.17 | | C |
| 10 | ATOM | 3372 | С | LYS A 214 | | 11.567 | 13.392 -11.355 | 1.00 54.17 | | 0 |
| | MOTA | 3373 | 0 | LYS A 214 | | 11.617 | 14.604 -11.251 | | | N. |
| | ATOM | 3374 | N | MET A 215 | | 12.632 | 12.628 -11.413 | 1.00 56.61 | | C |
| | MOTA | 3376 | CA | MET A 215 | | 13.932 | 13.165 -11.741 | 1.00 57.04 | • | c |
| | MOTA | 3378 | CB | MET A 215 | | 14.810 | 13.356 -10.511 | 1.00 57.19 | | c |
| 15 | MOTA | 3381 | CG | MET A 215 | | 14.273 | 14.458 -9.634 | 1.00 60.76 | | · s |
| | MOTA | 3384 | SD | MET A 215 | | 15.283 | 14.900 -8.238 | 1.00 63.39 | | C |
| | MOTA | 3385 | CE | MET A 215 | | 16.644 | 15.670 -9.212 | 1.00 63.56 | | c |
| | MOTA | 3389 | С | MET A 215 | | 14.534 | 12.189 -12.723 | 1.00 55.93 | | |
| • | MOTA | 3390 | 0 | MET A 215 | | 14.070 | 11.083 -12.896 | 1.00 51.96 | | 0 |
| 20 | MOTA | 3391 | N | ASP A 216 | | 15.562 | 12.614 -13.410 | 1.00 58.57 | | N |
| | ATOM | 3393 | CA | ASP A 216 | | 16.199 | 11.718 -14.331 | 1.00 62.39 | | C · |
| | ATOM | 3395 | CB | ASP A 216 | | 17.142 | 12.500 -15.225 | 1.00 64.34 | | C |
| | ATOM | 33.98 | CG | ASP A 216 | | 18.371 | 11.744 -15.547 | 1.00 62.34 | | C |
| | ATOM | 3399 | OD1 | ASP A 216 | | 18.562 | 10.659 -14.958 | 1.00 64.91 | • | 0 |
| 25 | ATOM | 3400 | OD2 | ASP A 216 | | 19.194 | 12.167 -16.384 | 1.00 69.70 | | 0 |
| | ATOM | 3401 | C | ASP A 216 | | 16.917 | 10.736 -13.424 | 1.00 63.11 | | C |
| | ATOM | 3402 | 0 | ASP A 216 | | 17.563 | 11.142 -12.458 | 1.00 62.81 | | 0 |
| | ATOM | 3403 | Ν. | CYS A 217 | | 16.824 | 9.446 -13.708 | 1.00 64.18 | | N |
| | ATOM | 3405 | CA | CYS A 217 | | 17.358 | 8.520 -12.735 | 1.00 66.46 | | C. |
| 30 | ATOM | 3407 | СВ | CYS A 217 | | 17.022 | 7.056 -13.051 | 1.00 66.11 | | C |
| 50 | ATOM | 3410 | SG | CYS A 217 | | 17.799 | 6.334 -14.479 | 1.00 72.28 | • | S |
| | ATOM | 3411 | С | CYS A 217 | | 18.822 | 8.755 -12.482 | 1.00 65.55 | | · C |
| | ATOM | 3412 | | CYS A 217 | | 19.283 | 8.527 -11.381 | 1.00 69.85 | | 0 |
| | ATOM | 3413 | N | LYS A 218 | | 19.547 | 9.255 -13.474 | 1.00 68.81 | | N |
| 35 | ATOM | 3415 | CA | LYS A 218 | ٠ | 20.992 | 9.436 -13.327 | 1.00 70.13 | | C |
| ,,, | ATOM | | СВ | LYS A 218 | | 21.618 | 10.160 -14.554 | 1.00 73.78 | | С |
| | ATOM | 3420 | CG | LYS A 218 | | 22.335 | 9.229 -15.609 | 1.00 76.00 | | C |
| | ATOM | 3423 | CD | LYS A 218 | | 23.033 | 9.987 -16.810 | 1.00 74.40 | | С |
| | ATOM | 3426 | CE | LYS A 218 | | 23.953 | 9.050 -17.717 | 1.00 75.92 | | C |
| 40 | ATOM | 3429 | NZ | LYS A 218 | | 23.299 | 7.995 -18.636 | 1.00 68.28 | | N |
| | ATOM | 3433 | С | LYS A 218 | | 21.288 | 10.204 -12.055 | 1.00 66.58 | | С |
| | ATOM | 3434 | ō | LYS A 218 | | 22.340 | 10.059 -11.456 | 1.00 68.40 | | 0 |
| | ATOM | 3435 | N . | GLU A 219 | | 20.347 | 11.014 -11.621 | 1.00 61.73 | | N |
| | ATOM | 3437 | CA | GLU A 219 | | 20.604 | 11.871 -10.482 | 1.00 61.25 | | C. |
| .45 | ATOM | 3439 | СВ | GLU A 219 | | 19.634 | 13.041 -10.528 | 1.00 60.32 | | С |
| . 43 | ATOM | 3442 | CG | GLU A 219 | | 19.746 | 13.887 -11.782 | 1.00 65.08 | | С |
| ÷ | ATOM | 3445 | CD | GLU A 219 | | 20.977 | 14.781 -11.827 | 1.00 65.35 | | С |
| | MOTA | | | L GLU A 219 | | 21.905 | 14.598 -10.998 | 1.00 62.03 | • | .0 |
| | MOTA | 3447 | | 2 GLU A 219 | | 21.001 | 15.673 -12.717 | 1.00 68.30 | - | 0 |
| 50 | | | C | GLU A 219 | | 20.493 | | 1.00 60.55 | | С |
| 50 | MOTA | 3449 | Ö | GLU A 219 | | 20.976 | 11.755 -8.113 | | | 0 |
| | ATOM | | N | TYR A 220 | | 19.848 | 10.055 -9.051 | | | N |
| | ATOM - | | | TYR A 220 | | 19.599 | 9.427 -7.771 | | | С |
| | ATOM | 3452 | CA | TYR A 220 | | 18.533 | | | | С |
| 55 | ATOM | 3454 | CB | TYR A 220 | | 17.175 | 8.915 -8.250 | | | С |
| 55 | MOTA | 3457 | CG | | • | 16.460 | 8.385 -9.284 | | | c |
| | ATOM | 3458 | | 1 TYR A 220 | | | 8.859 -9.601 | | | C |
| ٠. | ATOM | 3460 | CE | 1 TYR A 220 | | 15.232 | | , | | C |
| | MOTA | 3462 | CZ | TYR A 220 | | 14.696 | | | | ō |
| | ATOM | 3463 | | TYR A 220 | | 13.443 | | | | Č |
| 60 | MOTA | 3465 | CE | 2 TYR A 220 | | 15.390 | | | | · c |
| | MOTA | 3467 | CD | 2 TYR A 220 | | 16.619 | 9.943 -7.529 | ±.00 40.33 | | Ŭ |
| | | | | | | | | • | | |

| 5 | MOTA | 3469 | С | TYR | A 220 | | 20.844 | 8.778 | -7.324 | 1.00 55.05 | | | С |
|------|------|------|-----|-------|-------|---|-----------|---------|---------|------------|-----|-----|-----|
| | ATOM | 3470 | 0 | TYR | A 220 | | 21.101 | 8.684 | | 1.00 58.11 | | | |
| • | ATOM | 3471 | N | | A 221 | | 21.616 | 8.340 | -8.310 | 1.00 56.80 | | | N |
| | ATOM | 3473 | CA | ASN | A 221 | | 22.886 | 7.658 | -8.110 | 1.00 56.10 | | | С |
| | MOTA | 3475 | CB | ASN | A 221 | | 22.874 | 6.380 | -8.928 | 1.00 51.38 | | | č |
| 10 | ATOM | 3478 | CG | | A 221 | | 21.838 | 5.430 | -8.435 | | | | c |
| | ATOM | 3479 | | | A 221 | | , 21.923 | 4.970 | -7.294 | 1.00 53.01 | | | |
| | ATOM | 3480 | | | A 221 | | 20.830 | 5.136 | -9.272 | | | | 0 |
| | ATOM | 3483 | C | | A 221 | | 24.068 | 8.511 | | 1.00 50.76 | | | N |
| • | ATOM | 3484 | Ö | | A 221 | | | | -8.521 | 1.00 59.72 | | | C |
| 15 | ATOM | 3485 | N | | A 222 | | 25.123 | 7.989 | | 1.00 63.63 | | | 0 |
| 13 | ATOM | 3487 | CA | | A 222 | | 23.909 | 9.823 | -8.393 | 1.00 63.40 | | | N |
| | ATOM | | | | | | 24.919 | 10.707 | -8.917 | 1.00 63.06 | | | C. |
| | ATOM | 3489 | CB | | A 222 | | 24.506 | 12.178 | -9.007 | 1.00 68.66 | | | С |
| | | 3492 | CG | | A 222 | | 25,696 | 13.048 | -9.334 | 1.00 67.88 | | | С |
| 20 | ATOM | 3493 | | | A 222 | | 26.577 | | -10.333 | 1.00 72.26 | | | С |
| 20 | ATOM | 3495 | | | A 222 | | 27.666 | | -10.632 | 1.00 77.81 | | | С |
| | MOTA | 3497 | CZ | | A 222 | | 27.889 | 14.606 | -9.925 | 1.00 79.75 | | 1 | С |
| | ATOM | 3498 | ОН | | A 222 | | 28.992 | 15.374 | -10.239 | 1.00 83.62 | | 4 | 0 |
| | ATOM | 3500 | | | A 222 | | 27.018 | 14.993 | -8.917 | 1.00 75.27 | | | c · |
| | ATOM | 3502 | CD2 | TYR | A 222 | | 25.942 | 14.216 | -8.632 | 1.00 69.85 | | | C |
| 25 | MOTA | 3504 | С | TYR | A 222 | | 26.139 | 10.534 | -8.091 | 1.00 61.93 | | . , | c |
| | MOTA | 3505 | 0 | TYR | A 222 | | 26.223 | 10.993 | -6.934 | 1.00 51.08 | | | ō |
| | ATOM | 3506 | N | | A 223 | | 27.055 | 9.829 | -8.771 | 1.00 65.98 | | | N |
| | ATOM | 3508 | CA | | A 223 | | 28.389 | 9.416 | -8.349 | 1.00 58.22 | | | C |
| | ATOM | 3510 | CB | | A 223 | | ~ ~ ~ ~ ~ | 10.429 | -7.382 | 1.00 58.25 | • | | c |
| 30 | ATOM | 3513 | CG | | A 223 | • | 29.709 | | -6.239 | 1.00 64.15 | | | c |
| | ATOM | 3514 | | | A 223 | | 28.983 | 9.249 | -5.377 | 1.00 75.60 | | | |
| | ATOM | 3515 | | | A 223 | | 30.956 | 9.791 | -6.110 | | | | 0 |
| | ATOM | 3516 | C · | | A 223 | * | 28.238 | 7.959 | -7.885 | 1.00 56.47 | • | | 0 |
| | ATOM | 3517 | Ö | | A 223 | | 28.790 | | | 1.00 56.27 | | | C |
| 35 | ATOM | 3518 | N | | A 224 | | 27.463 | 7.052 | -8.514 | 1.00 48.60 | | | 0 |
| 55 | ATOM | 3520 | CA | | A 224 | | | 7.710 | -6.829 | 1.00 60.43 | | | N |
| | ATOM | 3522 | CB | | A 224 | | 27.203 | 6.317 | -6.389 | 1.00 58.39 | | | С |
| | ATOM | 3525 | CG | | A 224 | | 28.440 | 5.692 | -5.784 | 1.00 55.03 | | | С |
| | ATOM | 3528 | CD | | | | 28.722 | 6.175 | -4.403 | 1.00 53.98 | | | С |
| 40 | ATOM | 3531 | | | A 224 | | 30.039 | 5.591 | -3.910 | 1.00 51.13 | | | С |
| 70 , | | | CE | | A 224 | | 30.576 | 6.430 | -2.777 | 1.00 50.78 | | | С |
| | MOTA | 3534 | NZ | | A 224 | | 30.830 | 7.806 | -3.279 | 1.00 52.27 | | | N |
| | ATOM | 3538 | С | | A 224 | | 26.093 | 6.132 | -5.382 | 1.00 57.12 | | (| С |
| | MOTA | 3539 | 0 | | A 224 | | 25.621 | 7.085 | -4.735 | 1.00 59.55 | | (| 0 |
| 15 | ATOM | 3540 | N | | A 225 | | 25.697 | 4.870 | -5.246 | 1.00 56.45 | | | N |
| 45 | ATOM | 3542 | CA | | A 225 | | 24.636 | 4.461 | -4.316 | 1.00 52.86 | | . (| С |
| | MOTA | 3544 | CB | | A 225 | | 23.338 | 4.274 | | 1.00 50.03 | | (| С |
| | MOTA | 3547 | OG | | A 225 | | 22.661 | . 5.516 | -5.099 | 1.00 52.69 | . · | (| 0 |
| | MOTA | 3549 | С | SER | A 225 | | 25.040 | 3:197 | -3.570 | 1.00 48.24 | | . (| С |
| | MOTA | 3550 | 0 | SER | A 225 | | 25.422 | 2.202 | -4.180 | 1.00 48.80 | | . (| |
| ∵50 | MOTA | 3551 | N | ILE | A 226 | | 24.969 | 3.241 | -2.244 | 1.00 44.93 | | | N |
| | ATOM | 3553 | CA | ILE | A 226 | | 25.441 | | -1.454 | 1.00 37.58 | | | C |
| • | ATOM | 3555 | CB | | A 226 | | | 2.379 | -1.017 | 1.00 39.22 | | | C |
| ٠ | MOTA | 3557 | CG1 | | A 226 | | | 3.507 | -0.005 | 1.00 37.98 | | | C |
| | ATOM | 3560 | | | A 226 | | 28.301 | 3.756 | 0.555 | 1.00 34.23 | | | |
| 55 | ATOM | 3564 | | | A 226 | • | 27.756 | 2.690 | -2.212 | 1.00 34.23 | | | C. |
| • | ATOM | 3568 | C | | A 226 | | 24.632 | 1.817 | | | | | C |
| | ATOM | 3569 | ŏ | | A 226 | | 23.774 | | -0.239 | 1.00 38.95 | | | C |
| | ATOM | 3570 | | | A 227 | | | 2.567 | 0.185 | 1.00 47.23 | | | 2 |
| | ATOM | 3572 | | | | | 24.920 | 0.635 | 0.310 | 1.00 40.07 | | | Ŋ |
| 60 | ATOM | 3574 | | | A 227 | | 24.282 | 0.137 | 1.528 | 1.00 39.95 | | | C |
| 00 | | 3574 | | | A 227 | | 23.835 | -1.340 | 1.378 | 1.00 36.39 | | | С |
| | MOTA | 3310 | CGI | VAL . | A 227 | | 23.223 | -1.863 | 2.677 | 1.00 42.20 | | (| |
| | | | | | | | | | | | | | |

| | | 7 | | | | | | | | | | | | | | |
|-----------------|--------|--------------|----------|------|---|-----|---|----|--------------|----------------|----------------|---|----------------|---|---|--------|
| 5 | . ATOM | 3580 | | VAL | | | | | 852 | -1.446 | 0.279 | | 32.66 | | | С |
| • | MOTA | 3584 | С | VAL | | | • | | 298 | 0.175 | 2.644 | | 41.52 | | | C |
| | MOTA | 3585 | 0 | VAL | | | | | 400 | -0.407 | 2.485 | | 31.57 | | | 0 |
| | MOTA | 3586 | N | ASP | | | | | 951 | 0.813 | 3.768 | | 42.83 | | | N |
| | ATOM | 3588 | CA | ASP | | | | | . 934 | 0.901 | 4.892 | | 44.00 | | | C |
| 10 | ATOM | 3590 | CB | ASP | | | | | 926 | 2.001 | 4.665 | | 47.22 | | | C |
| | ATOM | 3593 | CG | ASP | | | | | .484 | 2.542 | 5.943 | | 55.34 | • | | C |
| | ATOM | 3594 | | ASP | | | | | .322 | 1.886 | 6.990 | | 60.37 | | | 0 |
| | MOTA | 3595 | OD2 | ASP | Α | 228 | | | .093 | 3.631 | 6.003 | | 65.03 | | | 0 |
| | ATOM | 3596 | С | ASP | | | | | . 364 | 1.037 | 6.287 | | 43.99 | | | C |
| 15 | ATOM | .3597 | 0 | ASP | | | | | 829 | 2.037 | 6.705 | | 43.43 | | | 0 |
| • | ATOM | 3598 | N | SER | | | | | . 535 | -0.057 | | | 45.99 | | | N |
| | MOTA | 3600 | CA | SER | | | | | .113 | -0.268 | 8.307 | | 43.77 | | | C |
| | MOTA | 3602 | CB | | | 229 | | | 400 | -1.715 | 8.589 | | 43.80 | | | Ċ |
| • | ATOM | 3605 | OG | SER | | | | | .786 | -1.836 | 8.462 | | 43.49 | | | 0 |
| 20 ⁻ | ATOM | 3607 | С | SER | | | | | . 987 | 0.478 | 9.228 | | 39.36 | | | C |
| | MOTA | 3608 | 0 | SER | | | | | .806 | 0.377 | 10.394 | | 35.35 | | | 0 |
| | MOTA | 3609 | N | GLY | | | | | .982 | 1.181 | 8.705 | | 40.62 | | • | N |
| | ATOM | 3611 | CA | GLY | | | | | . 805 | 2.105 | 9.509 | | 37.16 | | - | С |
| | MOTA | 3614 | С | GLY | | | | | .388 | 3.543 | 9.319 | | 38.50 | | | C |
| 25 | MOTA | 3615 | 0 | GLY | | | | | .040 | 4.500 | 9.740 | | 38.84 | | | 0 |
| | MOTA | 3616 | N | THR | | | | | .265 | 3.690 | 8.657 | | 36.83 | | | N |
| | MOTA | 3618 | CA | THR | | | | | . 672 | 4.981 | 8.477 | | 36.29 | | | С |
| | MOTA | 3620 | CB | THR | | | | | .795 | 5.339 | 7.037 | | 36.20 | | | С |
| | MOTA | 3622 | | THR | | | | | .141 | 5.728 | 6.829 | | 32.63 | | - | 0 |
| 30 | MOTA | 3624 | | THR | | | | | .980 | 6.570 | 6.709 | | 33.65 | | | C |
| | MOTA | 3628 | С | THR | | | | | .231 | 4.977 | 8.968 | | 36.96 | | • | Ċ |
| | MOTA | 3629 | 0 | THR | | | | | .479 | 4.036 | 8.702 | | 36.51 | | | 0 |
| | MOTA | 3630 | N | THR | | | | | .868 | 6.048 | 9.672 | | 39.63 | | | N |
| | ATOM | 3632 | CA | | | 232 | • | | .586 | 6.197 | 10.378 | | 44.48 | | | C C |
| 35 | ATOM | 3634 | СВ | THR | | | | | .776 | 7.362 | 11.370 | | 47.87 | | | 0 |
| | ATOM | 3636 | | THR | | | | | .819 | 7.053 | 12.305 | | 58.32 | | | C |
| • | ATOM | 3638 | | THR | | | | | .553 | 7.610 | 12.240 | | 52.16 | | | C |
| | MOTA | 3642 | С | THR | | | | | .384 | 6.554 | 9.507 | | 46.65 | | | 0. |
| 40 | ATOM | 3643 | 0 | THR | | | | | .315 | 5.954 7.547 | 9.593 8.663 | | 48.65 47.89 | | | N- |
| 40 | ATOM | 3644 | N | | | 233 | | | .590 | 8.231 | 7.983 | | 47.43 | | | C |
| | ATOM | 3646 | CA | ASN | | | | | .523 .878 | 9.715 | 7.971 | | 48.12 | | | C |
| | MOTA | 3648 | CB | ASN | | | | | | 10.435 | 9.198 | | 43.02 | | | č |
| | ATOM | 3651 | CG | ASN | | 233 | | | .435 .365 | 9.883 | 10.276 | | 38.96 | | | ŏ |
| 45 | ATOM | 3652 | | ASN | | | | | .145 | 11.703 | 9.035 | | 50.70 | | | Ŋ |
| 43 | MOTA . | 3653 | C | | | 233 | • | | .451 | 7.803 | 6.572 | | 48.67 | | | C |
| | ATOM | 3656 3657 | 0 | | | 233 | | | .360 | 7.093 | 6.131 | • | 51.81 | | | ō |
| | ATOM | | N | LEU | | | | | .403 | 8.234 | 5.856 | | 45.12 | | | N |
| | ATOM | 3658 | CA | | | 234 | | | .333 | 7.999 | | | 46.15 | , | | Ċ |
| 50 | MOTA | 3660 | CB | | | 234 | | | .912 | | 3.895 | | 46.39 | | | . c |
| 50 - | ATOM | 3662 | CG | | | 234 | | | | 7.785 | 2.424 | | 46.15 | | | C |
| | MOTA | 3665 | | LEU | | | | | .562 | 8.293 | | | 47.55 | | | , Ç |
| | MOTA | 3667 | | LEU | | | | | .868 | 7.415 | 1.522 | | 47.77 | • | · | Ċ |
| | ATOM | 3671 3675 | CDZ | | | 234 | • | | .842 | 9.286 | 3.867 | | 45.80 | | | ·c |
| 55 | ATOM | 3676 | o | | | 234 | | | .245 | 10.301 | 4.146 | | 51.40 | | | ŏ |
| 33 | MOTA | • | | | | 235 | | | .940 | 9.231 | 3.104 | | 47.98 | | | N |
| | ATOM | 3677 | N CA | | | 235 | • | | | 10.393 | 2.452 | | 41.53 | | | C |
| | ATOM | 3679 | CA CB | | | 235 | | | .555 .058 | 10.333 | 2.514 | | 40.87 | | | c |
| | ATOM | 3681 | CG. | | | 235 | | | .653 | 9.849 | | | 41.40 | • | | C |
| 60 | ATOM | 3684 | · CD | | | 235 | | | .645 | 10.825 | 4.775 | | 46.10 | | | c |
| 60 | ATOM | 3687 3690 | NE | | | 235 | | | .981 | 11.103 | 5.305 | | 52.10 | | | N |
| | ATOM | 3690 | rut, | נאוט | А | دري | | 24 | TOC. | | 3.303 | | 02.10 | | | •1 |
| | | | | | | | | | | | | | | | | |

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|-----|--------|--------|-----|-----------|---|---------|--------|---------|------|---------|---|---|---|----|
| 5 | ATOM | 3692 | CZ | ARG A 235 | | 25.469 | 12.342 | 5.380 | | 54.49 | | | | 2 |
| | ATOM | 3693 | NH1 | ARG A 235 | | 26.649 | 12.577 | 5.870 | | 51.49 | | | | N |
| | ATOM | 3696 | | ARG A 235 | | 24.751 | 13.366 | 4.949 | | 62.47 | | | | N |
| | ATOM | 3699 | | ARG A 235 | | 21.284 | 10.362 | 0.984 | | 42.47 | | | • | C |
| | | | | ARG A 235 | | 21.322 | 9.234 | 0.354 | 1.00 | 35.71 | | | (| 0 |
| •• | ATOM | 3700 | | LEU A 236 | | 21.054 | 11.575 | 0.446 | | 42.38 | | | 1 | N |
| 10 | ATOM | 3701 | | | | 20.755 | 11.710 | -0.959 | | 44.15 | | | (| C |
| | ATOM | 3703 | | LEU A 236 | | | | -1.112 | | 46.30 | | | | c |
| | MOTA | 3705 | | LEU A 236 | | 19.287 | 12.033 | | | | | | | c |
| | MOTA | 3708 | | LEU A 236 | | 18.420 | 11.070 | -0.325 | | 46.08 | | | | |
| | MOTA | 3710 | CD1 | LEU A 236 | | 17.143 | 11.742 | 0.192 | | 50.37 | | | , | Ç |
| 15 | ATOM | 3714 | CD2 | LEU A 236 | | 18.143 | 9.851 | -1.201 | | 46.39 | | | | С |
| 1.5 | ATOM | 3718 | | LEU A 236 | | 21.574 | 12.774 | -1.606 | 1.00 | 46.18 | | | | C |
| | | 3719 | _ | LEU A 236 | • | 21.974 | 13.760 | -1.003 | 1.00 | 56.50 | | | | 0 |
| | ATOM | | | PRO A 237 | | 21.861 | 12.556 | -2.850 | 1.00 | 43.50 | | | | N |
| | MOTA | 3720 | | | | 22.474 | 13.586 | -3.669 | | 48.09 | | | | С |
| | MOTA | 3721 | CA | PRO A 237 | | | | -5.075 | | 50.44 | | | | С |
| 20 | MOTA | 3723 | CB | PRO A 237 | | 22.378 | 13.003 | | | 47.91 | | | | Č. |
| | ATOM | 3726 | CG | PRO A 237 | | 22.263 | 11.517 | -4.873 | | | | | | Ċ |
| | ATOM . | 3729 | ĆD | PRO A 237 | | 21.677 | 11.287 | -3.541 | | 43.62 | | | | |
| | ATOM | 3732 | С | PRO A 237 | | 21.657 | 14.854 | -3.533 | | 47.59 | • | | | C |
| | ATOM | 3733 | 0 | PRO A 237 | | 20.443 | 14.793 | -3.621 | | 56.42 | | | | 0 |
| 25 | MOTA | 3734 | N | LYS A 238 | | 22.324 | 15.977 | ~3.340 | 1.00 | 54.44 | | | | N |
| 23 | ATOM | 3736 | CA | LYS A 238 | | 21.710 | 17.262 | -2.966 | 1.00 | 59.43 | | | | С |
| | | 3738 | CB | LYS A 238 | | 22.759 | 18.345 | -3.006 | 1.00 | 65.19 | | | | С |
| | ATOM | | | LYS A 238 | | 22.458 | 19.459 | -2.056 | 1.00 | 68.51 | | | | С |
| | ATOM | .3741 | CG | | | 21.616 | 20.524 | -2.702 | | 69.31 | | | | С |
| | ATOM | 3744 | CD | LYS A 238 | | | 21.491 | -1.626 | | 74.63 | | | | C |
| .30 | MOTA | 3747 | CE. | LYS A 238 | | 21.206 | | | | 72.38 | | | | Ň |
| | MOTA | 3750 | NZ | LYS A 238 | | 21.148 | 20.760 | -0.296 | | | | | | C |
| | MOTA | 3754 | С | LYS A 238 | | 20.530 | 17.740 | -3.770 | | 60.04 | | | | 0 |
| | ATOM | 3755 | 0 | LYS A 238 | | 19.535 | 18.188 | -3.218 | | 62.70 | | | | |
| | ATOM | 3756 | N | LYS A 239 | | 20.645 | 17.681 | -5.078 | | 61.99 | | | ~ | N |
| 35 | ATOM | 3758 | CA | LYS A 239 | | 19.502 | 17.942 | -5.889 | | 62.06 | | | • | С |
| 55 | ATOM | 3760 | СВ | LYS A 239 | | 19.803 | 17.627 | -7.373 | 1.00 | 65.93 | | | | С |
| | ATOM | 3763 | ČG | LYS A 239 | | 19.794 | 18:830 | -8.411 | 1.00 | 69.24 | | | | C. |
| | ATOM. | 3766 | CD | LYS A 239 | | 21.071 | 18.808 | -9.350 | 1.00 | 71.82 | | | | С |
| | | | CE | LYS A 239 | | 20.782 | | -10.877 | 1.00 | 73.55 | | | | С |
| 40 | ATOM | 3769 | | LYS A 239 | | 21.914 | | -11.760 | | 70.78 | | | | N |
| 40 | MOTA | 3772 | NZ | | | | 16.999 | -5.285 | | 64.24 | | | | С |
| | MOTA | 3776 | C | LYS A 239 | | 18.444 | | -4.781 | | 68.73 | | | | ō |
| | MOTA | 3777 | 0 | LYS A 239 | | 17.406 | 17.455 | | | | | | | N |
| | MOTA | 3778 | N | VAL A 240 | | 1,8.705 | 15.691 | -5.278 | | 58.91 | | | | C |
| | ATOM | 3780 | CA | VAL A 240 | | 17.635 | 14.751 | -4.914 | | 62.19 | | | | |
| 45 | MOTA | 3782 | CB | VAL A 240 | | 18.084 | 13.284 | -4.909 | | 65.97 | | | | C. |
| | ATOM | 3784 | CG1 | VAL A 240 | | 16.867 | 12.392 | -4.847 | 1,00 | 66.12 | | | | С |
| | ATOM | 3788 | | VAL A 240 | | 18.913 | 12.947 | -6.147 | 1.00 | 68.39 | | | | С |
| | MOTA | 3792 | C | VAL A 240 | | 17.034 | 15.079 | -3.556 | 1.00 | 58.68 | | | | С |
| | | | | VAL A 240 | | 15.811 | | -3.379 | 1.00 | 54.40 | | • | | 0 |
| ~^ | MOTA | 3793 | | VAL A 240 | | 17.906 | | -2.587 | | 56.41 | | | | N |
| 50 | ATOM | 3794 | N | PHE A 241 | | | | -1.278 | | 52.63 | | | | С |
| | MOTA | 3796 | CA | PHE A 241 | | | 15.677 | | | 50.48 | | • | | C |
| | MOTA | 3798 | CB | PHE A 241 | | 18.635 | | -0.376 | | | | | | Ċ |
| | MOTA | 3801 | CG | PHE A 241 | | 18.276 | | 0.957 | | 50.54 | | | | |
| | MOTA | . 3802 | CD1 | PHE A 241 | | 17.615 | | 1.945 | | 53.71 | | • | | C |
| 55 | MOTA | 3804 | | PHE A 241 | | 17.303 | 16.447 | 3.181 | | 54.61 | | | | С |
| 22 | ATOM - | 3806 | CZ | PHE A 241 | | 17.662 | | 3.427 | 1.00 | 55.24 | | | | С |
| | ATOM | 3808 | CES | PHE A 241 | | 18.322 | | 2.440 | | 55.17 | | | • | С |
| | | | | PHE A 241 | | 18.624 | | | | 57.01 | | | | C |
| | ATOM | 3810 | | PHE A 241 | | 16.561 | | | | 0 51.84 | | | | С |
| | ATOM | 3812 | | | | 15.439 | | | | 0 47.71 | | | | o |
| 60 | MOTA | 3813 | | PHE A 241 | | | | | | 0 53.89 | • | | | N |
| | ATOM | 3814 | N | GLU A 242 | | 17.031 | 17.857 | -2.243 | | 0 33.09 | • | | | ., |
| | | | | | | | | | | | | | | |

| 5 | ATOM | 3816 | CA | GLU . | A 242 | 1 | 6.239 | 19.085 | -2.353 | 1.00 | 56.53 | | | . C |
|----|--------------|--------------|----------|-------|----------------|-------|----------------|------------------|--------|------|----------------|---|----|-----|
| | MOTA | 3818 | CB | | A 242 | - · 1 | 6.797 | 20.110 | -3.362 | 1.00 | 59.79 | | • | C |
| | MOTA | 3821 | CG | | A 242 | 1 | 7.432 | 21.353 | -2.697 | 1.00 | 66.19 | | | С |
| | MOTA | 3824 | CD | | A 242 | | 7.130 | | -1.185 | 1.00 | 74.63 | | | С |
| •• | ATOM | 3825 | | GLU . | | | 5.931 | | -0.789 | 1.00 | 79.35 | | | 0 |
| 10 | MOTA | 3826 | | GLU . | | | 8.091 | | -0.372 | 1.00 | 76.40 | | | 0 |
| | ATOM | 3827 | C | | A 242 | | 4.790 | 18.768 | -2.638 | 1.00 | 53.63 | | | С |
| | ATOM | 3828 | 0 | | A 242 | | 3.937 | 19.203 | -1.880 | 1.00 | 45.24 | | | 0 |
| • | ATOM | 3829 | N | | A 243 | | 4.536 | | -3.709 | | 52.72 | | | N |
| 16 | ATOM | 3831 | CA | | A 243 | | 3.180 | | -4.140 | | 50.49 | | | C |
| 15 | ATOM | 3833 | CB | | A 243 | | 3.258 | 16.838 | -5.428 | | 51.48 | | | С |
| | MOTA | 3837 | C | | A 243 | | 2.383 | | -3.120 | | 51.02 | | | С |
| | ATOM | 3838 | 0 | | A 243 | | 1.259 | 17.157 | -2.763 | | 54.64 | | | 0 |
| | ATOM | 3839 | N | | A 244 | | 2,949 | | -2.653 | | 46.51 | | | N |
| 20 | MOTA MOTA | 3841 3843 | CA CB | | A 244 | | 2.262 | 14.833 | -1.670 | | 41.75 | • | | C |
| 20 | ATOM | 3847 | | ALA A | | | 3.173 | | -1.156 | | 37.69 | | | C |
| | ATOM | 3848 | C O | | A 244 A 244 | | 1.792 | 15.630 | -0.490 | | 44.76 | | | С |
| | ATOM | 3849 | N | | A 244 | | 0.658 | 15.496 | -0.084 | | 47.71 | | | 0 |
| | ATOM | 3851 | CA | | A 245 | | 2.646 | 16.470 | 0.083 | | 52.14 | | | N |
| 25 | ATOM | 3853 | CB | | A 245 | | 2.279 | 17.094 | 1.348 | | 53.69 | | | C |
| 23 | ATOM | 3855 | | VAL A | | | 3.325 2.824 | 18.100 | 1.854 | | 53.93 | | | C |
| | ATOM | 3859 | | VAL 2 | | | 1.659 | 18.785 | 3.121 | | 53.73 | | | C |
| | ATOM | 3863 | C | VAL A | | | 0.976 | 17.433 17.810 | 2.106 | | 58.55 | | | C |
| | ATOM | 3864 | Ö | | A 245 | | 0.072 | 17.775 | 1.141 | | 52.68 57.49 | | | C |
| 30 | ATOM | 3865 | N | LYS A | | |).904 | 18.444 | -0.015 | | 49.32 | | | 0 |
| | ATOM | 3867 | CA | LYS A | | | 9.816 | 19.327 | -0.367 | | 54.20 | | • | N |
| | ATOM | 3869 | СВ | LYS A | | | 200 | 19.988 | -1.684 | | 58.55 | | | C |
| | ATOM | 3872 | CG | LYS A | | | 1.763 | 19.868 | -1:943 | | 63.23 | , | | C |
| • | ATOM | 3875 | CD | LYS A | | | 2.640 | 21.041 | -1.337 | | 70.71 | | *. | C |
| 35 | ATOM | 3878 | CE | | 246 | | 3.228 | 20.765 | 0.055 | | 70.11 | | | C |
| | ATOM | 3881 | NZ | LYS A | | | 3.337 | 22.015 | 0.860 | | 70.79 | | | N |
| | ATOM | 3885 | С | LYS A | | | 3.550 | 18.497 | -0.458 | | 56.50 | , | | C |
| | MOTA | 3886 | 0 | LYS A | 4 246 | | 7.635 | 18.653 | 0.345 | | 62.61 | | | ŏ |
| | ATOM | 3887 | N | SER A | 4 247 | | 3.510 | 17.574 | -1.417 | | 53.80 | | | N |
| 40 | ATOM | 3889 | CA | SER A | 247 | 7 | 7.381 | 16.674 | -1.534 | | 45.07 | | | Ĉ |
| • | ATOM | 3891 | CB | SER A | 247 | 7 | 7.699 | 15.537 | -2.496 | | 45.02 | | | C |
| | ATOM | 3894 | OG | SER A | 247 | 6 | 5.636 | 14.587 | -2.462 | | 43.14 | | | 0 |
| • | ATOM | 3896 | С | SER A | 247 | 7 | 7.010 | 16.123 | -0.162 | | 38.07 | | | Ċ |
| | MOTA | 3897 | 0 | SER A | 4 247 | 5 | .842 | 15.925 | 0.137 | | 47.02 | | | 0 |
| 45 | ATOM | 3898 | N | ILE A | 248 | 8 | 8.008 | 15.906 | 0.685 | | 35.51 | | | N |
| | ATOM | 3900 | CA | ILE A | 248 | 7 | 7.738 | 15.379 | 2.012 | 1.00 | 44.04 | | | С |
| | ATOM | 3902 | СВ | ILE A | | | .068 | 14.787 | 2.672 | 1.00 | 45.65 | | | С |
| | MOTA | 3904 | | ILE A | | | .363 | 13.394 | 2.080 | 1.00 | 38.16 | • | | C |
| ~0 | MOTA | 3907 | | ILE A | | | 760 | 12.863 | 2.337 | 1.00 | 33.98 | | | ٠C |
| 50 | MOTA | 3911 | | ILE A | | 8 | .970 | . 14.588 | 4.187 | 1.00 | 46.92 | | | C |
| | MOTA | 3915 | С | ILE P | | | .955 | 16.401 | 2.846 | 1.00 | 51.15 | | • | С |
| | MOTA | 3916 | 0 | ILE A | | | 5.052 | 16.024 | 3.606 | 1.00 | 56.50 | | | 0 |
| | ATOM | 3917 | | LYS A | | | .281 | 17.689 | 2.671 | 1.00 | 53.92 | | | N |
| | ATOM | 3919 | | LYS A | | | 6.627 | 18.796 | 3.389 | 1.00 | 54.59 | | | C |
| 55 | ATOM | 3921 | | LYS A | | | .303 | 20.147 | | | 58.74 | | | С |
| | ATOM | 3924 | | LYS A | | | .585 | 20.554 | 3.850 | | 58.89 | | • | C |
| • | ATOM | 3927 | | LYS A | | | .099 | 21.880 | 3.249 | 1.00 | 58.57 | | | С |
| | MOTA | 3930 | | LYS A | | | .483 | 22.330 | 3.774 | | 61.39 | | | C |
| 60 | MOTA | 3933 | | LYS'A | | | .350 | 22.849 | 2.647 | | 57.83 | | | N |
| 60 | MOTA | 3937 | | LYS A | | | .177 | 18.935 | 2.964 | | 54.92 | | | С |
| : | MOTA | 3938 | 0 | LYS A | 249 | 4 | .246 | 18.932 | 3.790 | 1.00 | 54.00 | | | 0 |
| | | | | | | | | • | | | | | | |

| | | | | | | | | | | 46 50 | | | | | |
|------|-------|--------|-----|-------|--------|---|--------|--------|--------|------------|----|---|---|---|----|
| 5 | MOTA | 3939 | N | ALA A | 1 250 | | 5.003 | 19.083 | 1.656 | 1.00 49.70 | | | | | N |
| | ATOM | 3941 | CA | ALA A | 250 | | 3.688 | 19.218 | 1.060 | 1.00 52.00 | | | | | С |
| | ATOM | 3943 | CB | ALA A | A 250 | | 3.786 | 19.096 | -0.465 | 1.00 53.40 | | | | | C |
| | ATOM | 3947 | | | 250 | | 2.773 | 18.163 | 1.636 | 1.00 53.09 | | | | 1 | С |
| | | 3948 | | | A 250 | | 1.602 | 18.407 | 1.922 | 1.00 60.66 | | | | | 0 |
| 10 | ATOM | | | | A 251 | | 3.344 | 16.980 | 1.805 | 1.00 57.05 | | | | | N |
| 10 | MOTA | 3949 | | | | | 2.639 | 15.818 | 2.338 | 1.00 55.70 | | | | | C |
| | ATOM | 3951 | | | A 251 | | | | | 1.00 53.52 | | | | | Ċ |
| | MOTA | 3953 | | | A 251 | | 3.420 | 14.558 | 1.986 | 1.00 58.05 | | | | | |
| 1. 7 | ATOM | 3957 | С | ALA A | A. 251 | • | 2.404 | 15.877 | 3.856 | | | | | | |
| | ATOM | 3958 | 0 | ALA A | 4.251 | | 1,461 | 15.323 | 4.372 | 1.00 62.89 | | | | | 0 |
| 15 | ATOM- | 3959 | N | SER A | A 252 | | 3.281 | 16.529 | 4.590 | 1.00 59.77 | | | | | N. |
| | ATOM | 3961 | CA | SER A | A 252 | | 3.147 | 16.572 | 6.034 | 1.00 56.96 | | | | | С |
| | ATOM | 3963 | СВ | | A 252 | | 4.562 | 16.585 | 6.606 | 1.00 59.16 | • | | | | С |
| | ATOM | 3966 | OG | | A 252 | | 5.524 | 16.922 | 5.592 | 1.00 58.00 |) | | | | 0 |
| | | | | | A 252 | | 2.413 | 17.837 | 6.419 | 1.00 56.47 | | • | | | С |
| •• | MOTA | 3968 | C | | | | | 18.098 | 7.575 | 1.00 51.08 | | | | | 0 |
| 20 | ATOM | 3969 | 0 | | A 252 | | 2.110 | • | 5.401 | 1.00 59.93 | | | | | N |
| •• | ATOM | 3970 | N | | A 253 | | 2.089 | 18.610 | | 1.00 59.10 | | | | | C |
| | ATOM | 3972 | CA | | A 253 | | 1.690 | 20.003 | 5.568 | | | | | | C |
| | ATOM | 3974 | CB | | A-253 | | 1.581 | 20.643 | 4.173 | 1.00 57.63 | | | | | |
| | ATOM | . 3977 | OG | SER . | A 253 | | 1.316 | 22.026 | 4.257 | 1.00 55.7 | | | | | 0 |
| 25 | ATOM | 3979 | С | SER . | A 253 | | 0.484 | 20.373 | 6.441 | 1.00 60.1 | | | | | С |
| 23. | ATOM | 3980 | Ο. | | A 253 | | 0.075 | 21.526 | 6.428 | 1.00 59.1 | 1 | | | | 0 |
| | ATOM | 3981 | N | | A 254 | | -0.099 | 19.451 | 7.200 | 1.00 60.3 | 5 | | | | И |
| | | 3983 | CA | | A 254 | | -1.147 | 19.897 | 8.117 | 1.00 60.8 |) | | | | С |
| | MOTA | | CB | | A 254 | | -2.318 | 18.951 | 8.293 | 1.00 60.7 | l | | | | С |
| 20 | MOTA | 3985 | | | | | -1.905 | 17.797 | 9.043 | 1.00 56.7 | | | | | 0 |
| 30 | ATOM | 3987 | | | A 254 | | -2.858 | 18.465 | 6.955 | 1.00 60.7 | | | | | С |
| | ATOM | 3989 | | | A 254 | | • | | 9.435 | 1.00 64.5 | | | | | C |
| | ATOM | 3993 | C | | A 254 | | -0.473 | 20.059 | | 1.00 68.0 | | | - | | 0 |
| | MOTA | 3994 | 0 | | A 254 | | -1.121 | 20.164 | 10.478 | | | | | | N |
| | MOTA | 3995 | N | | A 255 | | 0.848 | 20.043 | | 1.00 66.3 | | | | | C |
| 35 | MOTA | 3997 | CA | | A 255 | | 1.626 | 20.400 | 10.537 | 1.00 69.5 | | | | | |
| | ATOM | 3999 | CB | GLU | A 255 | | 1.998 | 19.192 | 11.398 | 1.00 70.3 | | | | | C |
| | MOTA | 4002 | CG | GLU | A 255. | | 0.804 | 18.717 | 12.245 | 1.00 70.8 | | | | | C |
| | MOTA | 4005 | CD | GLU | A 255 | | 1.164 | 18.170 | 13.624 | 1.00 72.2 | | | | | С |
| | ATOM | 4006 | OE1 | GLU | A 255 | | 2.307 | 18.397 | 14.115 | 1.00 79,5 | | | | | 0 |
| 40 | ATOM | 4007 | OE2 | GLU | A 255 | | 0.285 | 17.519 | 14.229 | 1.00 62.9 | 3 | | | | 0 |
| | ATOM | 4008 | C | | A 255 | | 2.810 | 21.164 | 10.000 | 1.00 72.5 | 7 | | | | С |
| | ATOM | 4009 | ō | | A 255 | | 3.248 | 20.966 | 8.852 | 1.00 74.2 | 7 | | | | 0 |
| | | | N | | A 256 | | 3.298 | 22.083 | 10.818 | 1.00 72.1 | | | | | N |
| | ATOM | 4010 | | | A 256 | | 4.408 | 22.901 | 10.411 | 1.00 68.6 | | | | | С |
| 4 5 | MOTA | 4012 | CA | | | | 4.017 | 24.356 | 10.254 | 1.00 69.6 | | | | | С |
| 45 | ATOM | 4014 | CB | | A 256 | | | 24.580 | 9.037 | 1.00 76.5 | | | | | С |
| | MOTA | 4017 | CG | | A 256 | | 3.138 | | 7.737 | 1.00 70.9 | | | | | Č |
| | ATOM | 4020 | CD | | A 256 | | 3.813 | | | 1.00 79.2 | | | • | | c |
| | MOTA | 4023 | CE | | A 256 | • | 3.261 | 24.791 | 6.471 | | | | | | |
| | MOTA | 4026 | NZ | LYS | A 256 | | 2.321 | 23.945 | 5.676 | 1.00 79.7 | | | | | N |
| 50 | MOTA | 4030 | С | LYS | A 256 | | 5.429 | | 11.462 | 1.00 64.9 | | | | | С |
| • | MOTA | 4031 | 0 | LYS | A 256 | | 5.097 | 22.569 | 12.658 | 1.00 51.5 | | | | | 0 |
| | ATOM | 4032 | N | PHE | A 257 | | 6.664 | 22.674 | 10.972 | 1.00 61.7 | 3 | | | | N |
| | ATOM | 4034 | CA | | A 257 | | 7.826 | 22.397 | 11.762 | 1.00 60.9 | 9 | | | | С |
| | | 4036 | СВ | | A 257 | | 8.370 | | 11.354 | | 88 | | | | С |
| 55 | MOTA | | CG | | A 257 | | 7.338 | | 11.397 | • | | | | | ·C |
| 55 | MOTA | 4039 | | | | | | | 10.232 | | | | | | С |
| | ATOM | 4040 | | | A 257 | | 6.875 | | 10.232 | | | • | | | C |
| | MOTA | 4042 | | | A 257 | | 5.931 | | | | | | | | C |
| | ATOM | 4044 | CZ | | A 257 | | 5.447 | | 11.503 | | | | | | |
| | MOTA | 4046 | | | A 257 | | 5.910 | | | | | | | | C |
| 60 | MOTA | 4048 | CD2 | | A 257 | | 6.840 | | | | | | | | C |
| | ATOM | 4050 | С | PHE | A 257 | | 8.811 | 23.466 | 11.392 | 1.00 59. | 35 | | | | С |
| | | | | | | | | | | | | | | | |

| | | | | | | | | | | | | | | | _ |
|----|------|------|-----|-------|-------|---|----------------|--------|--------|------|---------|---|---|-----|-----|
| 5 | ATOM | 4051 | o | PHE A | 257 | | 8.716 | 24.049 | | | 58.22 | | | |) |
| | MOTA | 4052 | | PRO A | 258 | | 9.766 | 23.724 | 12.257 | | 61.91 | | | 1 | |
| | ATOM | 4053 | | PRO A | | | 10.792 | 24.731 | 11.983 | | 65.38 | | | | 3 |
| | MOTA | 4055 | | PRO A | | | 11.351 | 25.053 | 13.358 | 1.00 | 66.17 | | | . (| 3 |
| | | | | PRO A | | | 10.803 | 23.979 | 14.309 | 1.00 | 64.85 | | | | С |
| 10 | MOTA | 4058 | | PRO A | | | 9.949 | 23.054 | 13.546 | 1.00 | 61.29 | | | (| С |
| 10 | MOTA | 4061 | | | | | 11.875 | 24.094 | 11.144 | 1.00 | 69.63 | | | | C |
| | MOTA | 4064 | С | PRO A | | | | | 11.335 | 1 00 | 67.19 | | | | Ö |
| | MOTA | 4065 | - | PRO A | | | 12.156 | 22.912 | | | 74.52 | | | | N |
| | MOTA | 4066 | N . | ASP A | | | 12.485 | 24.858 | 10.248 | 1.00 | 76.21 | • | | | C |
| | MOTA | 4068 | | ASP A | | | 13.450 | 24.293 | 9.308 | 1.00 | 70.21 | | | | C · |
| 15 | MOTA | 4070 | CB | ASP A | 259 | | 14.038 | 25.411 | 8.459 | 1.00 | 78.78 | | | | |
| | ATOM | 4073 | CG | ASP A | 259 | | 12.952 | 26.362 | 7.934 | 1.00 | 85.56 | | | | C |
| | MOTA | 4074 | OD1 | ASP A | 259 | | 12.355 | 26.110 | 6.853 | | 85.56 | | | | 0 |
| | ATOM | 4075 | OD2 | ASP A | 259 | | 12.604 | 27.384 | 8.566 | 1.00 | 94.62 | | | | 0 |
| - | ATOM | 4076 | С | ASP F | | | 14.514 | 23.433 | 10.009 | | 75.34 | | | | С |
| 20 | ATOM | 4077 | ő | | 259 | | 14.811 | 22.315 | 9.560 | | 77.54 | | | , | O, |
| 20 | | 4078 | N | GLY A | 260 | | 15.056 | 23.927 | 11.119 | 1.00 | 68.42 | | | • | N |
| | ATOM | | CA | GLY A | | | 16.038 | 23.173 | 11.867 | | 65.64 | | | | С |
| | MOTA | 4080 | | GLY A | | - | 15.782 | 21.681 | 11.757 | | 64.85 | | | | С |
| | ATOM | 4083 | C | | | | 16.705 | 20.864 | 11.545 | | 65.50 | | | | 0 |
| | MOTA | 4084 | 0 | GLY A | | | | 21.331 | 11.912 | | 62.03 | | | | N |
| 25 | MOTA | 4085 | N | | 1 261 | | 14.512 | | 11.778 | | 60.14 | | | | C |
| | MOTA | 4087 | CA | | 261 | | 14.039 | 19.953 | | | 59.84 | | | | č |
| | MOTA | 4089 | CB | | A 261 | | 12.545 | 19.893 | 12.146 | | | | | | C |
| | MOTA | 4092 | CG | | A 261 | | 11.901 | 18.542 | 11.976 | | 53.88 | | | | Ċ |
| | MOTA | 4093 | CD1 | PHE A | A 261 | | 12.040 | 17.584 | 12.931 | | 50.78 | | | | |
| 30 | ATOM | 4095 | CE1 | PHE A | A 261 | | 11.450 | 16.369 | 12.790 | | 51.53 | | | | C |
| | ATOM | 4097 | CZ | PHE A | A 261 | | 10.699 | 16.096 | 11.676 | | 55.50 | • | | | С |
| • | ATOM | 4099 | CE2 | PHE A | A 261 | | 10.542 | 17.043 | 10.705 | | 51.48 | | | | С |
| | ATOM | 4101 | CD2 | PHE 2 | A 261 | | 11.140 | 18.260 | 10.859 | | 55.00 | | | | С |
| | ATOM | 4103 | C | | A 261 | | 14.271 | 19.432 | 10.364 | 1.00 | 60.30 | | | | С |
| 35 | ATOM | 4104 | ō | | A 261 | | 14.921 | 18.396 | 10.165 | 1.00 | 62.84 | | | | 0 |
| 55 | MOTA | 4105 | N · | | A 262 | | 13.778 | 20.132 | 9.363 | 1.00 | 52.97 | - | | | N |
| | | | CA | | A 262 | | 13.930 | 19.551 | 8.071 | | 54.85 | | | | C |
| | MOTA | 4107 | CB | | A 262 | | 13.154 | 20.339 | 7.017 | 1.00 | 56.23 | | | | С |
| | ATOM | 4109 | | | | • | 11,652 | 20.135 | 7.269 | | 61.23 | | | | С |
| 40 | ATOM | 4112 | CG | | A 262 | | 10.780 | 21.050 | 7.761 | | 66.49 | | | | С |
| 40 | ATOM | 4113 | | | A 262 | | | 20.510 | 7.874 | | 68.50 | | | | N |
| | MOTA | 4115 | | | A 262 | | 9.525 9.565 | | 7.447 | | 67.88 | | | | С |
| | MOTA | 4117 | | | A 262 | | | 19.213 | 7.064 | | 61.30 | | | • | Č |
| | MOTA | 4118 | | | A 262 | | 10.889 | 18.941 | | | 64.17 | | | | Č |
| , | MOTA | 4119 | | | A 262 | • | 11.188 | 17.669 | 6.586 | | | | | | c |
| 45 | ATOM | 4121 | | | A 262 | | 10.177 | 16.728 | 6.510 | | 63.85 | - | | | č |
| | MOTA | 4123 | | | A 262 | • | 8.879 | 17.034 | 6.896 | • | 66.57 | | | | |
| | MOTA | 4125 | CZ2 | TRP | A 262 | | 8.547 | 18.266 | | | 66.36 | | • | | C |
| | ATOM | 4127 | Ċ | TRP | A 262 | | 15.391 | 19.391 | 7.785 | | 53.56 | | | | C |
| | MOTA | 4128 | 0 | TRP | A 262 | | 15.769 | 18.849 | 6.757 | 1.00 | 56.81 | | | | 0 |
| 50 | ATOM | 4129 | N. | LEU | A 263 | | 16.220 | | 8.725 | 1.00 | 58.44 | | | | N |
| 30 | MOTA | 4131 | CA | | A 263 | | 17.677 | | 8.531 | 1.00 | 58.98 | | | | С |
| | | 4133 | СВ | | A 263 | | 18.170 | | | | 57.08 | | | | С |
| | ATOM | | | | A 263 | | 18.031 | | 7.709 | | 59.71 | | | - | С |
| | MOTA | 4136 | | | | | 18.483 | | 8.206 | | 59.96 | | | | С |
| | ATOM | 4138 | | | A 263 | - | 18.875 | | 6.527 | | 60.81 | | | | C |
| 55 | MOTA | 4142 | | | A 263 | | | | 9.398 | | 0 62.54 | | | | c |
| | MOTA | 4146 | | | A 263 | | 18.468 | | | | | | | | o |
| | ATOM | 4147 | | | A 263 | - | 19.686 | | 9.526 | | 0 61.58 | | | | |
| | MOTA | 4148 | N | | A 264 | | 17.778 | | 10.012 | | 0 67.37 | | | | N |
| | MOTA | 4150 | CA | | A 264 | | 18.436 | | | | 0 70.18 | | | | C |
| 60 | ATOM | 4153 | | GLY | A 264 | | 18.788 | | 12.179 | | 0 72.26 | | | | C |
| | ATOM | 4154 | | GLY | A 264 | | 18.910 | 17.143 | 13.194 | 1.0 | 0 76.04 | | | | 0 |
| | | | | | | | | | | | | | | | |

| | | | | | | | | | | | | | | | 1.7 |
|---------|-------|------|----------------|----------------|-----|----|--------|--------|--------|-------|------------------|---|---|---|--------|
| 5 | ATOM. | 4155 | | GLU A 2 | | | 18.927 | 19.149 | 12.149 | | 71.01 | | | | N C |
| | MOTA | 4157 | CA . | GLU A 2 | 265 | • | 19.437 | | 13.311 | | 71.40 | | • | | C. |
| | ATOM | 4159 | СВ | GLU A 2 | 265 | | 19.648 | 21.383 | | | 71.95 | | | | |
| | ATOM | 4162 | CG | GLU A 2 | 265 | | 20.982 | 21.698 | 12.353 | | 74.37 | | | | C |
| | ATOM | 4165 | CD | GLU A 2 | 265 | | 20.958 | 22.955 | 11.471 | | 74.89 | | | | C |
| 10 | ATOM | 4166 | | GLU A | | | 21.757 | 23.022 | 10.500 | | 63.91 | | | | 0 |
| 10 | ATOM | 4167 | | GLU A | | | 20.142 | 23.876 | 11.745 | | 80.45 | | | | 0 |
| | ATOM | 4168 | С | GLU A | | | 18.592 | 19.716 | 14.547 | | 70.60 | | | | С |
| | ATOM | 4169 | ō | GLU A | | | 19.099 | 19.216 | 15.542 | 1.00 | 72.28 | | | | 0 |
| | ATOM | 4170 | N . | GLN A | | • | 17.322 | 20.118 | 14.516 | | 68.36 | | | | N |
| 1 5 | ATOM | 4172 | CA | GLN A | | | 16.574 | 20.094 | 15.769 | | 68.13 | | | | С |
| 15 | MOTA | 4174 | СВ | GLN A | | | 16.036 | 21.431 | 16.254 | 1.00 | 71.81 | | | | С |
| | | 4177 | CG | GLN A | | | 15.288 | 22.275 | 15.282 | 1.00 | 73.46 | | | | С |
| | ATOM | 4180 | CD | GLN A | | | 15.211 | 23.702 | 15.831 | 1.00 | 80.14 | | | | С |
| • | ATOM | | | GLN A | | | 16.098 | 24.530 | 15.578 | 1.00 | 78.16 | | | | 0 |
| .00 | ATOM | 4181 | | GLN A | | | 14.163 | 23.982 | 16.604 | | 81.99 | | | | N |
| 20 | MOTA | 4182 | | GLN A | | | 15.495 | 19.132 | 15.770 | | 65.19 | | | | С |
| | ATOM | 4185 | C | | | | 14.952 | 18.739 | 14.761 | | 68.32 | | | | 0 |
| | MOTA | 4186 | 0 | GLN A LEU A | | | 15.179 | 18.751 | 16.973 | | 62.13 | | | | N |
| | MOTA | 4187 | N | | | | 14.400 | 17.604 | 17.135 | | 60.81 | | | | С |
| | MOTA | 4189 | | LEU A | | | 14.990 | 16.849 | 18.335 | | 60.23 | | | | С |
| 25 | MOTA | 4191 | CB | LEU A | | | | 17.271 | 19.724 | | 56.50 | | | | C |
| | MOTA | 4194 | CG | LEU A | | | 14.662 | 17.340 | 19.756 | | 54.80 | | | | С |
| | ATOM | | | LEU A | | | 13.130 | 16.210 | 20.656 | | 52.66 | | | | C |
| | MOTA | 4200 | | LEU A | | | 15.234 | | 17.205 | | 60.54 | | | • | С |
| | MOTA | 4204 | C · | LEU A | | | 12.988 | 18.098 | 17.203 | | 67.47 | | | | ō |
| 30 | ATOM | 4205 | 0 | LEU A | | | 12.771 | 19.279 | | | 67.35 | | | | N |
| | MOTA | 4206 | N | VAL A | | | 12.013 | 17.214 | 17.315 | | 64.13 | | | | C |
| | MOTA | 4208 | CA | VAL A | | | 10.617 | 17.635 | 17.398 | | 64.12 | | | | c |
| | MOTA | 4210 | CB | VAL A | | | 9.915 | 17.517 | 16.071 | | | | | | Ċ. |
| | MOTA | 4212 | | VAL A | | ٠. | 8.431 | 17.553 | 16.280 | | . 64.85 68.52 | | | | Ċ. |
| 35 | MOTA | 4216 | CG2 | VAL A | | | 10.332 | 18.629 | 15.148 | | | | | | c |
| | MOTA | 4220 | С | VAL A | | | 9.895 | 16.719 | 18.348 | | 65.02 | | | | Ö |
| | MOTA | 4221 | · O | VAL A | | | 10.339 | 15.595 | 18.595 | | 67.72 | | | | N |
| | MOTA | 4222 | N _. | CYS A | | | 8.774 | 17.185 | 18.876 | | 64.09 | | | | C |
| | MOTA | 4224 | CA | CYS A | | | 8.045 | 16.373 | 19.822 | | 64.62 | | | | c |
| 40 | MOTA | 4226 | CB | CYS A | 269 | | 8.506 | 16.794 | 21.203 | | 66.31 | | | | s |
| | MOTA | 4229 | SG | CYS A | 269 | | 10.286 | 17.212 | 21.240 | | 69.02 | | | | C |
| | ATOM | 4230 | С | CYS A | | | 6.523 | 16.452 | 19.735 | | 64.55 | | | | |
| | ATOM | 4231 | 0 | CYS A | 269 | | 5.943 | 17.350 | | | 67.95 | | | | 0 |
| | ATOM | 4232 | N | TRP A | 270 | | 5.899 | 15.479 | | | 61.04 | | | | N |
| 45 | ATOM | | CA | TRP A | | | 4.444 | 15.334 | 20.512 | | 61.84 | | | | C |
| | ATOM | 4236 | CB | TRP A | 270 | | 3.764 | 14.554 | | • . | 56.93 | | | | . C |
| | ATOM | 4239 | CG | TRP . A | 270 | | 3.867 | 15.143 | 17.967 | | 58.64 | | | · | C |
| | ATOM | 4240 | CD1 | TRP A | 270 | | 3.041 | 16.067 | 17.388 | | 59.48 | | | | С |
| | ATOM | 4242 | NE3 | TRP A | | | 3.452 | 16.344 | 16.105 | | 54.79 | | | | N |
| 50 | ATOM | 4244 | | TRP A | | | 4.562 | | 15.825 | 1.00 | 57.15 | | | | С |
| , ,0 | | 4245 | | TRP A | | | 4.848 | | 16.971 | | 56.20 | • | | | С |
| | MOTA | 4246 | | TRP A | | | 5.948 | | | 1.00 | 49.93 | | | | С |
| | ATOM | 4248 | | TRP A | | | 6.708 | | | | 55.27 | | | | √, C |
| | ATOM | | | TRP A | | | 6.395 | | | | 58.79 | | | | C |
| <i></i> | ATOM | 4250 | CZ | | | | 5.331 | | | | 55.58 | | | | С |
| 55 | ATOM | 4252 | | | | | 4.288 | | | | 64.90 | | | | · C |
| | MOTA | 4254 | ·C | TRP A | | | 5.212 | | | | 0 64.95 | | | • | 0 |
| | MOTA | 4255 | 0 | TRP A | | | | | | | 0 64.50 | | | | N |
| | MOTA | 4256 | N | GLN A | | | 3.112 | | | | 0 59.95 | | | | С |
| | ATOM | 4258 | CA | GLN A | | • | 2.891 | | | | 0 58.83 | | | | Č |
| 60 | ATOM | 4260 | | GLN A | | | 1.547 | | | | 0 65.33 | | | | C |
| | MOTA | 4263 | CG | GLN A | 271 | | 1.117 | 10.042 | 23.773 | , 1.0 | | | | | _ |

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                    CA
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                   CA
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                                                 11.277
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              4365 ND2 ASN A 278
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                                                 10.409
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      MOTA
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| Ė | 3 mos4 | 4370 | | TTE 8 2 | 70 | | 0.154 | 11.459 | 9.136 | 1.00 | 45.86 | | | N |
|-----|--------|-------|-----|---------|------|----|------------------|--------|------------------|------|-------|---|--|---|
| · 5 | ATOM | 4370 | | ILE A 2 | | | 0.262 | 12.647 | 8.283 | | 40.58 | | | С |
| | MOTA | 4372 | | ILE A 2 | | | 0.202 | 13.912 | 9.019 | | 41.95 | | | Ċ |
| | MOTA | 4374 | | ILE A 2 | | | 1.508 | 14.087 | 9.747 | | 44.28 | | | Ċ |
| | MOTA | 4376 | | ILE A 2 | | | | 15.503 | 10.041 | | 48.63 | | | Č |
| 40. | ATOM | 4379 | | ILE A 2 | | | 1.810 | 13.936 | 9.940 | | 40.98 | | | C |
| 10 | MOTA | 4383 | | ILE A 2 | | | -1.078 | | 7.511 | | 41.25 | | | c |
| | MOTA | 4387 | С | ILE A 2 | | | 1.502 | 12.647 | 6.527 | | 41.55 | | | o |
| | MOTA | 4388 | | ILE A 2 | | | 1.571 | 13.405 | | | 42.95 | | | N |
| | MOTA | 4389 | N | PHE A 2 | | | 2.494 | 11.830 | 7.932 | | 43.36 | | | C |
| | MOTA | 4391 | | PHE A 2 | | | 3.734 | 11.696 | 7.155 | | 47.33 | | | c |
| 15 | MOTA | 4393 | CB | PHE A 2 | | | 4.914 | 11.371 | 8.031 | | 48.46 | | | c |
| | ATOM | 4396 | CG | PHE A 2 | | | 5.285 | 12.438 | 9.006 | | 52.35 | | | C |
| | ATOM | 4397 | | PHE A 2 | | | 6.155 | 13.457 | 8.641 | | | | | Ċ |
| | ATOM | 4399 | | PHE A 2 | | | 6.512 | 14.437 | 9.555 | | 55.06 | | | C |
| | MOTA | 4401 | CZ | PHE A 2 | | | 5.997 | 14.385 | 10.859 | | 53.18 | | | C |
| 20 | MOTA | 4403 | | PHE A 2 | | | 5.131 | 13.352 | 11.213 | | 48.87 | , | | C |
| | ATOM | 4405 | CD2 | PHE A 2 | | | 4.791 | 12.401 | 10.296 | | 47.29 | | | |
| | ATOM | 4407 | C | PHE A 2 | 280 | | 3.596 | 10.572 | 6.116 | | 43.82 | | | C |
| • | ATOM | 4408 | 0 | PHE A 2 | 280 | | 2.937 | 9.572 | 6.344 | | 46.62 | | | 0 |
| | ATOM | 4409 | N | PRO A 2 | 281 | | 4.236 | 10.726 | 4.978 | | 41.27 | | | N |
| 25 | ATOM | 4410 | CA | PRO A 2 | 281 | | 4.127 | 9.768 | 3.874 | | 35.61 | | | С |
| | ATOM . | 4412 | СВ | PRO A | 281 | | 4.376 | 10.655 | 2.660 | | 36.29 | | | С |
| | ATOM | 4415 | CG | PRO A | 281, | | 5.171 | 11.767 | 3.144 | | 35.91 | | | С |
| | MOTA | 4418 | CD | PRO A | 281 | | 5.116 | 11.847 | 4.657 | | 37.67 | | | C |
| | ATOM | 4421 | С. | PRO A | | | 5.217 | 8.679 | 3.868 | | 39.20 | | | С |
| 30 | ATOM | 4422 | 0 | PRO A | | | 6.162 | 8.792 | 4.650 | 1.00 | 35.73 | | | 0 |
| | ATOM | 4423 | N | VAL A | | | 5.072 | 7.679 | 2.981 | 1.00 | 36.56 | | | N |
| | ATOM | 4425 | CA | VAL A | | | 5.987 | 6.562 | 2.819 | | 35.89 | | | C |
| | ATOM | 4427 | СВ | VAL A | 282 | | 5.215 | 5.282 | 2.365 | 1.00 | 39.74 | | | С |
| | ATOM | 4429 | | VAL A | | | 4.205 | 4.818 | 3.377 | 1.00 | 36.87 | | | С |
| 35 | ATOM | 4433 | | VAL A | | | 4.500 | 5.499 | 1.028 | 1.00 | 45.22 | | | С |
| 55 | ATOM | 4437 | C | VAL A | • | ** | 7.030 | 6.872 | 1.714 | 1.00 | 40.69 | | | С |
| | ATOM | 4438 | ō | VAL A | | | 6.797 | 7.738 | 0.873 | 1.00 | 36.67 | | | Ò |
| | ATOM | 4439 | N | ILE A | | | 8.156 | 6.136 | 1.705 | 1.00 | 37.84 | | | N |
| | MOTA | 4441 | CA | ILE A | | | 9.241 | 6.356 | 0.712 | 1.00 | 38.96 | | | С |
| 40 | ATOM | 4443 | СВ | ILE A | | | 10.411 | 7.053 | 1.374 | 1.00 | 38.64 | | | С |
| ••• | ATOM | 4445 | | ILE A | | | 9.963 | 8.318 | 2.070 | 1.00 | 44.14 | | | С |
| | ATOM | 4448 | | ILE A | | | 11.109 | 9.046 | 2.658 | 1.00 | 48.84 | | | С |
| | ATOM | 4452 | | ILE A | | | 11.481 | 7.314 | 0.311 | 1.00 | 29.11 | | | С |
| | ATOM | 4456 | C | ILE A | | | 9.899 | 5.255 | -0.053 | 1.00 | 41.40 | | | С |
| 45 | MOTA | 4457 | Ö | ILE A | | | 10.851 | 4.668 | 0.441 | 1.00 | 62.61 | | | 0 |
| 773 | MOTA | 4458 | N | SER A | | | 9.483 | | -1.293 | 1.00 | 44.38 | | | N |
| | MOTA | 4,460 | CA | SER A | | | 9.856 | 3.861 | -2.002 | 1.00 | 41.93 | | | С |
| | MOTA | 4462 | CB | SER A | | | 8.683 | 3.407 | -2.819 | 1.00 | 42.78 | | | С |
| | ATOM | 4465 | OG | SER A | | | 7.555 | 3.197 | -1.991 | | 44.75 | | | 0 |
| 50 | ATOM | 4467 | C | SER A | | | 11.040 | 4.075 | -2.897 | | 44.34 | | | С |
| 50 | | 4468 | Ö | SER A | | | 11.022 | 4.922 | -3.788 | | 46.55 | | | Ó |
| | MOTA | | • | LEU A | | | 12.090 | 3.315 | -2.656 | | 41.54 | | | N |
| | ATOM | 4469 | N | | | | 13.223 | 3.384 | -3.521 | | 37.02 | | | С |
| | MOTA | 4471 | CA | LEU A | | | 14.491 | 3.276 | -2.717 | | 35.95 | | | C |
| | ATOM | 4473 | CB | LEU A | | | | 4.402 | -1.704 | | 38.01 | | | C |
| 55 | MOTA | 4476 | CG | LEU A | | | 14.805 16.196 | 4.144 | -1.122 | | 33.26 | | | C |
| | ATOM | 4478 | | LEU A | | | | | -2.251 | | 33.20 | | | c |
| • | MOTA | 4482 | | LEU A | | | 14.762 | 5.845 | -2.251 -4.451 | | 38.43 | | | C |
| | MOTA | 4486 | С | LEU A | | | 13.043 | 2.195 | | | 30.43 | | | ō |
| | MOTA | 4487 | 0 | LEU A | | | 12.880 | 1.086 | | | 32.94 | | | N |
| 60 | MOTA | 4488 | N | TYR A | | | 13.017 | 2.399 | -5.759 | | | | | C |
| | MOTA | 4490 | CA | TYR A | 286 | | 12.855 | 1.262 | -6.641 | 1.00 | 39.45 | | | C |

| 5 | ATOM | 4492 | СВ | TYR A | 286 | 17.11.3 1.011 7.010 | C |
|------|--------|------|------|-------|--------|------------------------------------|--------|
| 5 | ATOM | 4495 | CG | TYR A | | 10.014 1.145 1.02. | C |
| | ATOM | 4496 | | TYR A | | 10.023 .2.010 0.330 1.00 | С |
| | ATOM | 4498 | | TYR A | | | C |
| | ATOM | 4500 | CZ | TYR F | A 286 | 7.894 1.996 -7.713 1.00 | C |
| 10 | MOTA | 4501 | OH | TYR F | | 0.310 2.13/ /.032 1.00 0 | 0 |
| 10 | MOTA | 4503 | | TYR F | | 0.4/0 1.130 0.301 1.00 | C |
| | MOTA | 4505 | | TYR A | | 9.021 1.025 0.040 2.00 | C |
| | ATOM | 4507 | С | | A 286 | 14.207 0.832 -7.119 1.00 36.96 | C |
| | MOTA | 4508 | Ο· | TYR A | A 286 | 14.990 1.054 -7.405 1.00 | 0 |
| 15 | MOTA | 4509 | N . | LEU A | A 287 | 14.465 -0.461 -7.177 1.00 37.56 | N C |
| | ATOM | 4511 | CA | LEU A | A 287 | 15.786 -0.941 -7.545 1.00 36.13 | C |
| | ATOM | 4513 | CB | LEU I | A 287 | 16.385 -1.695 -6.391 1.00 37.50 | C |
| | ATOM | 4516 | CG | LEU A | A 287 | 16.513 -1.001 -5.061 1.00 40.67 | c |
| • | MOTA | 4518 | | LEU A | | 16.957 -2.079 -4.008 1.00 42.47 | c |
| 20 | MOTA | 4522 | CD2 | LEU I | | 17.507 0.090 -5.144 1.00 37.99 | c |
| | ATOM . | 4526 | С | LEU I | A 287 | 15.760 -1.869 -8.700 1.00 32.81 | 0 |
| | ATOM | 4527 | 0 | LEU I | A 287 | 14.789 -2.561 -8.889 1.00 42.24 | N |
| | ATOM | 4528 | N | | A 288 | 16.849 -1.897 -9.447 1.00 37.48 | |
| | MOTA | 4530 | CA | MET I | A 288 | 17.040 -2.777 -10.632 1.00 43.22 | C C |
| 25 - | ATOM | 4532 | CB | MET 7 | A 288 | 18.349 -2.356 -11.349 1.00 49.18 | c |
| | ATOM | 4535 | CG | MET . | A 288 | 19.046 -3.419 -12.208 1.00 53.21 | S |
| | ATOM | 4538 | SD | MET . | A 288 | 20.373 -2.706 -13.301 1.00 68.95 | |
| | ATOM | 4539 | CE | MET | A 288 | 19.993 -0.904 -13.311 1.00 59.14 | C |
| | MOTA | 4543 | С | MET | A 288 | 17.104 -4.269 -10.276 1.00 42.94 | C |
| 30 | ATOM | 4544 | 0 | MET | A 288 | 17.771 -4.671 -9.328 1.00 46.50 | O N |
| | MOTA | 4545 | N | GLY | A 289 | 16.446 -5.098 -11.055 1.00 40.57 | |
| | ATOM | 4547 | CA | GLY | A 289 | 16.290 -6.485 -10.682 1.00 43.24 | C C |
| • | ATOM | 4550 | С | GLY | A 289 | 17.409 -7.294 -11.225 1.00 48.62 | 0 |
| | ATOM- | 4551 | 0 | GLŸ | A 289 | 18.320 -6.726 -11.761 1.00 57.55 | N |
| -35 | MOTA | 4552 | N | | A 290 | | C |
| , | ATOM | 4554 | CA | | A 290 | | C |
| | MOTA | 4556 | CB | | A 290 | | C |
| | MOTA | 4559 | CG | | A 290 | | c |
| | MOTA | 4562 | CD | | A 290 | | 0 |
| 40 | MOTA | 4563 | OE l | GLU | A 290 | 19.365 -12.576 -8.331 1.00 47.44 | ŏ |
| | MOTA | 4564 | OE2 | | A 290 | | c |
| | ATOM ' | 4565 | С | GLU | A 290 | 17.928 -9.808 -13.091 1.00 63.07 | ö |
| | MOTA | 4566 | 0 | | A 290 | | N |
| | MOTA | 4567 | N | | A 291 | | C |
| 45 | ATOM | 4569 | CA | | A 291 | | č |
| | ATOM | 4571 | CB | VAL | A 291 | 14.926 -10.790 -14.824 1.00 64.54 | c |
| | MOTA | 4573 | | | A 291 | | č |
| | MOTA . | 4577 | ··CG | | A 291 | | č |
| | MOTA | 4581 | С | | A 291 | | ő |
| 50 | MOTA | 4582 | 0 | | A 291 | | N |
| | ATOM | 4583 | N | | A 292 | | C. |
| | ATOM | 4585 | CA | | A 292 | | č |
| | MOTA | 4587 | CB | THR | A 292 | | o. |
| | MOTA | 4589 | OG | 1 THR | A 292 | | C |
| 55 | MOTA | 4591 | CG | | A 292 | | · C |
| | MOTA | 4595 | С | | A 292 | | 0 |
| | MOTA | 4596 | 0 | | A 292 | | N |
| | ATOM | 4597 | N | | A 293 | | C |
| | ATOM | 4599 | CA | | A 293 | | C |
| 60 | ATOM | 4601 | CB | | `A 293 | | C |
| | MOTA | 4604 | CG | GLN | A 293 | 3 12.971 -5.013 -19.979 1.00 69.90 | C |
| | | | | | | · | |

| 5 | ATOM | 4607 | CD | GLN F | A 293 | | 13.563 | -3.662 | -19.780 | | 73.82 | | | С |
|------|------|------|-----|-------|---------|----|--------|---------|---------|------|-------|-----|-----|-----|
| • | MOTA | 4608 | | GLN F | A 293 | | 14.704 | -3.406 | -20.178 | 1.00 | 76.41 | | | 0 |
| | ATOM | 4609 | NE2 | GLN A | A 293 | ;- | 12.804 | -2.784 | -19.105 | 1.00 | 70.84 | | | N |
| | ATOM | 4612 | С | GLN A | A 293 | | 13.057 | -4.736 | -16.364 | 1.00 | 63.03 | | | С |
| | ATOM | 4613 | 0 | GLN A | A 293 | | 12.284 | -3.803 | -16.127 | 1.00 | 67.21 | | | 0 |
| 10 | ATOM | 4614 | | | A 294 | | 13.367 | -5.661 | -15.484 | 1.00 | 57.71 | | | N |
| | MOTA | 4616 | | GLN A | A 294 | | 12.562 | -5.859 | -14.307 | 1.00 | 56.14 | | | С |
| | ATOM | 4618 | | GLN A | A 294 | | 12.735 | -7.332 | -13.870 | 1.00 | 56.19 | | | С |
| | ATOM | 4621 | CG | | A 294 | | 11.579 | -7.951 | -13.090 | 1.00 | 56.15 | | | С |
| | ATOM | 4624 | CD | GLN A | A 294 | | 11.247 | -9.407 | -13.475 | 1.00 | 55.02 | | | C. |
| 15 | ATOM | 4625 | | | A 294 | | | -10.255 | | 1.00 | 46.01 | | | 0 |
| 10 | ATOM | 4626 | | | A 294 | | 11.271 | | -14.777 | 1.00 | 49.71 | | | N. |
| | ATOM | 4629 | С | | A 294 | | 13.045 | -4.905 | -13.257 | 1.00 | 51.59 | | | С |
| | ATOM | 4630 | 0 | GLN A | A 294 | | 14.132 | -4.397 | -13.369 | 1.00 | 50.97 | | | 0 |
| • | ATOM | 4631 | N | | A 295 | | 12.229 | | -12.260 | 1.00 | 47.06 | | | N |
| 20 | ATOM | 4633 | CA | | A 295 | | 12.740 | -3.950 | -11.063 | 1.00 | 48.50 | | | С |
| 20 | ATOM | 4635 | CB | | A 295 | | 12.882 | -2.483 | -11.321 | 1.00 | 42.42 | | | С |
| | ATOM | 4638 | OG | | A 295 | | 11.655 | -2.067 | -11.834 | 1.00 | 48.16 | | | 0 |
| | ATOM | 4640 | C | | A 295 | | 11.773 | -4.171 | -9.895 | 1.00 | 46.17 | | | С |
| | ATOM | 4641 | Ō | | A 295 | | 10.676 | | -10.059 | 1.00 | 48.16 | | | 0 |
| -25 | ATOM | 4642 | N | | A 296 | | 12.146 | | -8.721 | 1.00 | 37.72 | | | N |
| ر بـ | ATOM | 4644 | CA | | A 296 | | 11.236 | -3.922 | -7.615 | 1.00 | 39.89 | | | C |
| | ATOM | 4646 | СВ | | A 296 | | 11.533 | -5.236 | -6.978 | 1.00 | 39.36 | | | С |
| | ATOM | 4649 | CG | | A 296 | | 12.886 | -5.286 | -6.295 | 1.00 | 32.98 | | | С |
| | ATOM | 4650 | | | A 296 | | 13.035 | -4.863 | -5.018 | 1.00 | 37.10 | | | С |
| 30 | MOTA | 4652 | | | A 296 | | 14.225 | -4.924 | -4.406 | 1.00 | 36.18 | | | C. |
| 50 | ATOM | 4654 | CZ | | A 296 | | 15.301 | -5.395 | -5.076 | 1.00 | 38.32 | | | C |
| | ATOM | 4656 | | | A 296 | | 15.172 | -5.807 | -6.332 | 1.00 | 36.15 | | | С |
| - | ATOM | 4658 | | | A 296 | | 13.969 | -5.760 | -6.939 | 1.00 | 29.00 | • | | C |
| | ATOM | 4660 | C | | A 296 | | 11.426 | -2.840 | -6.592 | 1.00 | 39.38 | | | Ċ. |
| 35 | ATOM | 4661 | ō | | A 296 | | 12.431 | -2.151 | -6.656 | 1.00 | 41.20 | | | 0 |
| | ATOM | 4662 | N | | A 297 | | 10.485 | -2.688 | -5.654 | 1.00 | 37.55 | | | N |
| | MOTA | 4664 | CA | ARG . | A 297 | | 10.624 | -1.626 | -4.641 | 1.00 | 38.59 | | | С |
| | MOTA | 4666 | CB | ARG . | A 297 | | 9.581 | -0.566 | -4.833 | 1.00 | 38.15 | | | C |
| | ATOM | 4669 | CG | ARG . | A 297 | | 8.264 | -0.977 | -4.508 | 1.00 | 37.91 | | | C |
| 40 | ATOM | 4672 | CD | ARG | A 297 | | 7.234 | -0.020 | -5.035 | 1.00 | 42.44 | | | C |
| | MOTA | 4675 | NE | | A 297 | | 5.889 | -0.478 | -4.612 | 1.00 | 45.80 | | • | N |
| • | ATOM | 4677 | CZ | ARG | A 297 | | 4.753 | -0.271 | -5.262 | 1.00 | 40.89 | | | С |
| | ATOM | 4678 | NH1 | ARG | A 297 | | 4.710 | 0.368 | -6.409 | 1.00 | 50.48 | | | N |
| | MOTA | 4681 | | | A 297 | | 3.650 | -0.712 | -4.767 | 1.00 | 38.31 | | | N |
| 45 | ATOM | 4684 | С | | A 297 | | 10.560 | -1.944 | -3.197 | 1.00 | 34.05 | | | C |
| | MOTA | 4685 | · 0 | ARG | A 297 | | 9.901 | -2.904 | | 1,00 | 38.82 | | | 0 |
| | ATOM | 4686 | N | ILE | A 298 | | 11.224 | -1.092 | -2.432 | 1.00 | 34.02 | | | N |
| | MOTA | 4688 | CA | ILE | A 298 | | 11.194 | -1.240 | | 1.00 | 33.72 | | | C |
| | MOTA | 4690 | СВ | ILE | A 298 · | | 12.584 | -1.357 | -0.399 | 1.00 | 35.84 | | | C. |
| 50 | MOTA | 4692 | | | A 298 | | 13.586 | -0.429 | -1.006 | 1.00 | 40.04 | | | C |
| | ATOM | 4695 | CD1 | ILE | A 298 | | 15.017 | -0.629 | -0.399 | 1.00 | 38.54 | | | C |
| | ATOM | 4699 | | | A 298 | | 13.234 | -2.643 | -0.863 | 1.00 | 40.77 | | | C |
| | ATOM | 4703 | С | ILE | A 298 | | 10.474 | -0.050 | -0.493 | 1.00 | 33.09 | | | С |
| | ATOM | 4704 | ο . | | A. 298 | | 10.772 | | -0.956 | 1.00 | 35.93 | • | | . 0 |
| 55 | | 4705 | N | | A 299 | | 9.508 | | | 1.00 | 38.13 | | • • | N |
| | ATOM | 4707 | CA | | A 299 | | 8.788 | | | 1.00 | 39.87 | | • | C |
| | ATOM | 4709 | СВ | | A 299 | | 7.268 | | | 1.00 | 41.38 | • | | С |
| | ATOM | 4711 | | | A 299 | | 6.955 | | | 1.00 | 41.84 | | | 0 |
| | ATOM | 4713 | | | A 299 | | 6.519 | | | 1.00 | 38.29 | | | С |
| 60 | ATOM | 4717 | C | | A 299 | | 9.017 | | | 1.00 | 39.18 | | | С |
| | ATOM | 4718 | ō | | A 299 | | 8.719 | | | | 42.23 | | | 0 |
| | | | - | | | | | | • | | | . • | | |

| | | • | | | | | | | | | | | | |
|------|--------|------|-----|-------|-----|----|----------|--------|---------|------|-------|---|---|-----|
| 5 | ATOM | 4719 | N | ILE A | 300 | | 9.561 | 2.371 | 2.818 | 1.00 | | | | N |
| _ | MOTA | 4721 | CA | ILE A | 300 | ٠. | 9.712 | 2.602 | 4.257 | | 43.86 | | | C . |
| | MOTA | 4723 | CB | ILE A | 300 | | 11.112 | 3.118 | 4.717 | 1.00 | | | | C |
| | ATOM | 4725 | CG1 | ILE A | 300 | | 11.584 | 4.378 | 4.011 | 1.00 | | | | C |
| | MOTA | 4728 | CD1 | ILE A | 300 | | 12.548 | 5.177 | 4.939 | 1.00 | | | | C · |
| 10 | MOTA | 4732 | CG2 | ILE A | 300 | | 12.167 | 2.091 | 4.499 | 1.00 | | | | C |
| | ATOM | 4736 | С | ILE A | 300 | | 8.619 | 3.494 | 4.769 | 1.00 | | | | С |
| • | MOTA | 4737 | 0 | ILE A | 300 | | 7.878 | 4.094 | 4.001 | 1.00 | | | | 0 |
| | ATOM | 4738 | N | LEU A | 301 | | 8.538 | 3.556 | 6.089 | 1.00 | | | | N |
| | MOTA | 4740 | CA | LEU A | 301 | | 7.515 | 4.294 | 6.798 | 1.00 | | | | Ċ |
| 15 | ATOM | 4742 | CB | LEU A | 301 | | 6.837 | 3.315 | 7.759 | 1.00 | | | | ·C· |
| | MOTA | 4745 | CG | LEU A | 301 | | 6.052 | 2.205 | 7.119 | 1.00 | | | | С |
| | ATOM | 4747 | CD1 | LEU A | 301 | | 5.467 | 1.524 | 8.188 | | 30.86 | | | C |
| | ATOM | 4751 | CD2 | LEU A | 301 | | 4.968 | 2.698 | 6.252 | | 34.38 | | | C, |
| • | ATOM | 4755 | С | LEU A | 301 | | 8.106 | 5.431 | 7.632 | | 39.51 | | | C |
| 20 | ATOM | 4756 | 0 | LEU A | 301 | | 9.292 | 5.472 | 7.850 | | 44.43 | | | 0 |
| | MOTA | 4757 | N | PRO A | 302 | | 7.286 | 6.338 | 8.142 | | 38.79 | | | N |
| , | MOTA | 4758 | CA | PRO A | 302 | | 7.819 | 7.393 | 9.001 | | 36.78 | | | С |
| | MOTA | 4760 | CB | PRO A | 302 | | 6.590 | 8.187 | 9.424 | 1.00 | 37.00 | | | С |
| | ATOM | 4763 | CG | PRO A | 302 | | 5.410 | 7.604 | 8.714 | 1.00 | 36.36 | | | С |
| 25 | ATOM | 4766 | CD | PRO A | 302 | | 5.832 | 6.424 | 7.958 | 1.00 | 36.66 | | | С |
| | ATOM | 4769 | С | PRO A | 302 | | 8.510 | 6.797 | 10.226 | | 38.02 | | | С |
| | ATOM | 4770 | 0 | PRO A | | | 9.516 | 7.327 | 10.642 | | 33.13 | | | 0 |
| | MOTA | 4771 | N | GLN A | 303 | | 7.995 | 5.719 | 10.811 | | 38.55 | | | N |
| | MOTA | 4773 | CA | GLN A | | | 8.699 | 5.129 | 11.945 | | 36.57 | | | С |
| 30 | ATOM - | 4775 | CB | GLN A | | | 8.003 | 3.902 | 12.457 | | 35.69 | | | С |
| - | ATOM | 4778 | CG | GLN A | 303 | | 6.751 | 4.170 | 13.195 | | 42.25 | • | | C . |
| | MOTA | 4781 | CD | GLN A | | | 5.602 | 4.274 | 12.297 | | 34.75 | | | С |
| | MOTA | 4782 | OE1 | GLN A | 303 | | 5.772 | 4.591 | 11.130 | | 46.30 | | | 0 |
| | ATOM | 4783 | | GLN A | | | 4.416 | 4.026 | 12.820 | | 42.67 | | | N |
| 35 | , ATOM | 4786 | С | GLN A | | | - 10.113 | 4.672 | 11.588 | | 42.43 | | | С |
| | ATOM | 4787 | 0 | GLN A | 303 | | 10.807 | 4.115 | 12.404 | | 44.66 | | | 0 |
| | ATOM | 4788 | N. | GLN A | 304 | | 10.554 | 4.872 | 10.373 | | 44.05 | | | N |
| | ATOM | 4790 | CA | GLN A | 304 | | 11.919 | 4.525 | 10.089 | | 43.84 | | | C |
| | ATOM | 4792 | CB | GLN A | 304 | | 12.025 | 3.506 | 8.939 | | 44.50 | | | С |
| 40 | ATOM | 4795 | CG | GLN A | 304 | | 11.789 | 2.069 | 9.464 | | 40.62 | | | C |
| | ATOM | 4798 | CD | GLN A | 304 | | 10.436 | 1.517 | 9.204 | | 41.50 | | | C |
| | MOTA | 4799 | OE1 | GLN A | 304 | | 9.915 | 0.808 | 10.039 | | 46.70 | | | 0 |
| | MOTA | 4800 | NE2 | GLN A | 304 | | 9.849 | 1.830 | 8.050 | | 43.88 | | | N |
| | MOTA | 4803 | С | GLN A | 304 | | 12.735 | 5.769 | 9.864 | | 43.47 | | | С |
| 45 | ATOM | 4804 | 0 | GLN A | 304 | | 13.806 | 5.890 | 10.460 | | 57.31 | | | 0 |
| • | MOTA | 4805 | N | TYR A | 305 | | 12.253 | 6.709 | 9.056 | • . | 43.84 | | | N |
| | MOTA | 4807 | CA | TYR A | | | 13.030 | 7.931 | 8.789 | | 42.11 | | | C |
| | MOTA | 4809 | CB | TYR A | 305 | | 12.741 | | 7.383 | | 42.55 | | | C |
| | ATOM | 4812 | CG | TYR A | 305 | | 11.329 | 9.026 | 7.065 | | 38.35 | | | C |
| . 50 | MOTA | 4813 | CD1 | TYR A | 305 | | 10.846 | 10.230 | 7.553 | | 39.92 | | | C |
| | MOTA | 4815 | CE1 | TYR A | 305 | | 9.579 | 10.679 | 7.245 | | 38.06 | | | C |
| | MOTA | 4817 | CZ | TYR A | 305 | | 8.745 | 9.931 | . 6.432 | | 44.35 | | • | C |
| | ATOM | 4818 | OH | TYR A | 305 | ٠. | 7.445 | 10.380 | 6.121 | | 47.26 | | | 0 |
| | MOTA | 4820 | CE2 | TYR A | 305 | | 9.206 | 8.737 | 5.934 | | 41.55 | | | C. |
| 55 | ATOM | 4822 | | TYR A | | | 10.502 | 8.296 | 6.252 | | 39.60 | | | C |
| , | MOTA | 4824 | С | TYR A | | | 12.920 | 8.991 | 9.901 | | 42.17 | | | С |
| | ATOM | 4825 | 0 | TYR F | | | 13.587 | 10.034 | 9.828 | | 47.00 | | | 0 |
| | ATOM | 4826 | N | LEU F | | | 12.096 | 8.727 | 10.910 | | 38.60 | | • | N |
| | ATOM | 4828 | CA | LEU A | | | 11.947 | 9.618 | | | 42.86 | | | , C |
| 60 | ATOM | 4830 | СВ | LEU A | | | 10.473 | 9.989 | 12.345 | 1.00 | 38.48 | | | C |
| | АТОМ | 4833 | CG | LEU A | | | 9.755 | 11.015 | 11.422 | 1.00 | 39.42 | | | С |
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11.981
                                                                 1.00 36.26
                                                                                        С
                                                11.473
                                        8:401
     MOTA
            4835
                  CD1 LEU A 306
                                                                                        С
                                                                 1.00 36.89
                                       10.561
                                                12:258
                                                         11.132
                  CD2 LEU A 306
    ATOM
            4839
                                                                                        C
                                                                 1.00 48.77
                       LEU A 306
                                                         13.236
                                       12.538
                                                 8.831
     MOTA
             4843
                   C
                                                                1.00 51.36
                                                                                        0
                                                         13.807
                       LEU A 306
                                       11.887
                                                 7.927
             4844
                   0
     MOTA
                                                                 1.00 47.61
                                                         13.589
                                                 9.181
                                       13.770
                       ARG A 307
     MOTA
             4845
                  N
                                                                                        С
                                                                 1.00 47.50
                                                         14.583
                                                 8.445
                       ARG A 307
                                       14.523
             4847
                   CA
10
     MOTA
                                                                                        C
                                                         14.079
                                                                 1.00 46.68
                                                 8.359
                                       15.977
                       ARG A 307
             4849
                   CB
     MOTA
                                                                                        C
                                                                 1.00 41.90
                                                 8.267
                                                         15.066
                       ARG A 307
                                       17.104
     MOTA
             4852
                   CG
                                                                 1.00 41.76
                                                                                        C
                                       18.410
                                                 8.260
                                                         14.346
                       ARG A 307
             4855
                   CD
     ATOM
                                                                 1.00 42.84
                                                                                       . N
                                                         14.580
                       ARG A 307
                                        19.209
                                                 9.451
                   NE
     ATOM
             4858
                                                                 1.00 42.66
                                                                                        C
                                                         15.767
                       ARG A 307
                                        19.635
                                                 9.809
             4860
                   CZ
15
     MOTA
                                                                  1.00 44.80
                                                                                        N
                                                         16,827
                   NH1 ARG A 307
                                                 9.068
                                        19.325
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| | MOTA | 5051 | CA | LYS A 3 | | | 15.025 | 13.851 | 14.547 | 1.00 49.46 | *** | |
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| | MOTA | 5056 | CG | LYS A 3 | 321 ' | | 17.182 | 15.141 | 15.141 | 1.00 53.31 | | C |
| | ATOM ' | 5059 | CD | LYS A | 321 | | 18.714 | 15.093 | 14.895 | 1.00 53.64 | | С |
| 10 | MOTA | 5062 | CE | LYS A | 321 | | 19.429 | 16.349 | 15.512 | 1.00 55.80 | | С |
| 10 | ATOM | 5065 | NZ | LYS A | | | 20.917 | 16.178 | 15.790 | 1.00 57.93 | | N |
| | | 5069 | | LYS A | | | 14.857 | 13.255 | 13.163 | 1.00 43.54 | | С |
| | MOTA | | Ö | LYS A | | | 14.681 | 12.069 | 13.016 | 1.00 49.60 | | 0 |
| | MOTA | | | PHE A | | | 14.947 | 14.097. | 12.161 | 1.00 41.25 | * | N |
| | MOTA | 5071 | N | PHE A | | | 14.655 | 13.750 | 10.791 | 1.00 43.43 | | С |
| - 15 | MOTA | 5073 | CA | | | · | 14.199 | 15.061 | 10.075 | 1.00 45.65 | | С |
| | ATOM | 5075 | CB | PHE A | | | | 14.910 | 8.629 | 1.00 41.86 | | C |
| | ATOM | 5078 | CG. | PHE A | | | 13.807 | | 8.257 | 1.00 41.79 | | C |
| | MOTA | 50 79 | | PHE A | | | 12.758 | 14.134 | | 1.00 37.29 | | Č. |
| | MOTA | 5081 | | PHE A | | | 12.427 | 14.000 | 6.960 | 1.00 37.23 | | C |
| 20 | MOTA | 5083 | CZ | PHE A | | | 13.125 | 14.653 | 5.982 | | | č |
| | ATOM | 5085 | | PHE A | | | 14.158 | 15.436 | 6.310 | 1.00 42.54 | | c |
| | ATOM | 5087 | CD2 | PHE A | 322 | | 14.509 | 15.566 | 7.642 | 1.00 46.49 | | c |
| | MOTA | 5089 | С | PHE A | 322 | | 15.961 | 13.138 | 10.239 | 1.00 48.97 | | |
| | MOTA | 5090 | 0 | PHE A | 322 | | 16.981 | 13.817 | 10.014 | 1.00 48.91 | | 0 |
| 25 | ATOM | 5091 | N | ALA A | | | 15.922 | 11.831 | 10.036 | 1.00 42.08 | | N |
| 23 | ATOM | 5093 | CA | ALA A | | | 17.072 | 11.115 | 9.597 | 1.00 39.45 | | С |
| | ATOM | 5095 | CB | ALA A | | | 17.011 | 9.753 | 10.228 | 1.00 38.16 | | С |
| | ATOM | 5099 | C. | ALA A | | | 17.297 | 11.012 | 8.047 | 1.00 42.70 | | С |
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| 20 | ATOM | 5101 | N | ILE A | | | 16.914 | 12.027 | 7.268 | 1.00 39.06 | | N |
| 30 | ATOM | | CA | ILE A | | | 17.177 | 11.971 | 5.799 | | | С |
| | ATOM | 5103 | | ILE A | | | 15.911 | 12.049 | 4.976 | 1.00 35.33 | | Ċ |
| | MOTA | 5105 | CB | | | | 15.063 | 10.826 | 5.158 | 1.00 41.82 | | С |
| | MOTA | 5107 | | ILE A | | | | 10.854 | 4.283 | 1.00 45.15 | | C |
| | ATOM | 5110 | | ILE A | | | 13,800 | | 3.553 | 1.00 39.72 | | c |
| 35 | ATOM | 5114 | | ILE A | | | 16.241 | 12.092 | 5.453 | 1.00 33.72 | | Ċ |
| | ATOM | 5118 | C | ILE A | | | 18.000 | 13.179 | | 1.00 47.75 | | o · |
| | MOTA | 5119 | 0 | ILE A | | | 17.491 | 14.268 | 5.571 | 1.00 47.73 | | N |
| | MOTA | 5120 | N | SER A | | | 19.244 | 13.022 | 5.011 | 1.00 47.83 | | C |
| | ATOM | 5122 | CA | SER A | | | 20.148 | | | | | C _. |
| 40 | ATOM | 5124 | CB | SER A | | | 21.194 | 14.129 | 5.977 | 1.00 51.02 | | 0 |
| | MOTA | 5127 | OG | SER A | 325 | | 21.991 | 12.978 | 5.786 | 1.00 60.15 | | C |
| | ATOM | 5129 | С | SER A | 325 | | 20.831 | 14.230 | 3.573 | 1.00 44.39 | | |
| | MOTA | 5130 | 0 | SER A | 325 | | 20.699 | 13.316 | 2.780 | 1.00 51.62 | | . 0 |
| | ATOM | 5131 | N | GLN A | 326 | | 21.579 | 15.286 | 3.320 | 1.00 49.08 | | N |
| 45 | ATOM | 5133 | CA | GLN A | 326 | | 22.095 | 15.527 | 1.954 | 1.00 50.41 | | C |
| | MOTA | 5135 | CB | GLN A | 326 | | 21.980 | 17.004 | 1.575 | 1.00 50.65 | | C |
| | ATOM | 5138 | ĊĠ | GLN A | | | 22.818 | 17.900 | 2.410 | 1.00 59.27 | | C |
| | ATOM | 5141 | CD | GLN A | | | 22.308 | 19.336 | 2.379 | 1.00 69.60 | * | C |
| | ATOM | 5142 | | L GLN A | | | 22.805 | 20.165 | 1.608 | 1.00 81.67 | | Ο. |
| 50 | | 5143 | | GLN A | | | 21.315 | 19.636 | 3.215 | 1.00 74.53 | | N |
| υŅ | MOTA | 5146 | | GLN A | | | 23.522 | 15.036 | 1.838 | 1.00 47.73 | | С |
| | ATOM | | | | | | 24.139 | 14.823 | 2.858 | 1.00 39.28 | | Ō |
| | MOTA | 5147 | O. | GLN A | | | 24.135 | 14.838 | | | | N |
| ** | ATOM | 5148 | N | SER A | | | | | 0.407 | 1.00 48.29 | | С |
| | MOTA | 5150 | CA | | | | 25.349 | 14.191 12.660 | | | | c |
| 55 | ATOM | 5152 | CB | SER A | | | 25.170 | | | | | ő |
| | ATOM | 5155 | | SER A | | | 26.109 | 11.808 | | | | . C |
| | MOTA | 5157 | | SER A | | | 26.057 | 14.402 | | | | 0 |
| | MOTA | 5158 | | SER A | | | 25.440 | 14.385 | | | | N |
| | ATOM | 5159 | | SER A | | | 27.375 | 14.538 | | | | C |
| 60 | ATOM | 5161 | | SER A | 328 | | 28.228 | 14.891 | | | | |
| | ATOM | 5163 | CB | SER A | 328 | | 29.294 | 15.862 | -1.479 | 1.00 59.74 | | С |
| | | | | | | | | | | | | |

| | | | | | | | • | | | | | | _ |
|----------|--------------|----------------|---------|--------------|----|--------|---------|---------|-------|---------|----|---|-----|
| 5 | MOTA | 5166 | OG | SER A 328 | | 30.068 | 15.264 | -0.446 | 1.00 | 58.39 | | | 0 |
| 3 | ATOM | 5168 | C | SER A 328 | | 28.901 | 13.650 | -2.507 | 1.00 | 63.61 | | | С |
| | ATOM | 5169 | ō | SER A 328 | | 29.458 | 13.656 | -3.630 | 1.00 | 62.54 | | | 0 |
| | ATOM | 5170 | N | THR A 329 | | 28.861 | 12.588 | -1.696 | 1.00 | | | | N |
| | ATOM | 5172 | CA | THR A 329 | | 29.372 | 11.305 | -2.132 | 1.00 | | | | С |
| 10 | | 5174 | СВ | THR A 329 | | 30.254 | 10.683 | -1.073 | 1.00 | | | | С |
| 10 | ATOM | 5176 | | THR A 329 | | 29.635 | 10.794 | 0.212 | | 56.80 | | | Ο. |
| | ATOM | 5178 | | THR A 329 | | 31.542 | 11.477 | -0.972 | 1.00 | 61.68 | | | С |
| | ATOM | 5182 | C | THR A 329 | | 28.280 | 10.328 | -2.543 | 1.00 | 55.97 | | | С |
| | MOTA | 5183 | o´ | THR A 329 | | 28.473 | 9.113 | -2.470 | | 61.73 | | | 0 |
| 15 | MOTA | 5184 | N | GLY A 330 | • | 27.131 | | -2.965 | 1.00 | 52.78 | | | Ν. |
| 15 | MOTA | 5186 | CA | GLY A 330 | | 26.102 | 9.994 | -3.558 | 1.00 | 47.81 | | | С |
| | MOTA MOTA | 5189 | C | GLY A 330 | ٤, | 05 070 | 9.508 | -2.565 | 1.00 | 40.66 | | | C. |
| | | 5190 | o | GLY A 330 | | 25.057 | 9.994 | -1.446 | | 41.70 | | | 0 |
| 4 | MOTA | 5191 | N | THR A 331 | | 24.242 | 8.545 | -2.962 | | 37.29 | | | N |
| 20 | MOTA | 5193 | CA | THR A 331 | | 23.170 | 8.072 | -2.094 | 1.00 | 37.86 | | | С |
| 20 | MOTA | 5195 | CB | THR A 331 | | 22.068 | 7.313 | -2.904 | 1.00 | 39.26 | | | С |
| | MOTA | | | THR A 331 | | 21.479 | 8.139 | -3.916 | 1.00 | 39.31 | | | 0 |
| | MOTA | 5197 | | THR A 331 | | 20.888 | 7.049 | -2.051 | | 42.31 | | | С |
| | MOTA | 5199 | C | THR A 331 | | 23.756 | 7.124 | -1.078 | 1.00 | 39.73 | | | С |
| 25 | MOTA | 5203 | 0 | THR A 331 | | 24.660 | 6.353 | -1.407 | 1.00 | 44.56 | | | 0 |
| 25 | MOTA | 5204 5205 | | VAL A 332 | | 23.258 | 7.178 | 0.154 | 1.00 | 40.26 | | | N |
| | MOTA | | N CA | VAL A 332 | | 23.641 | 6.187 | 1.152 | 1.00 | 35.90 | ٠. | | С - |
| | ATOM | 5207 5200 | CB | VAL A 332 | | 24.604 | 6.690 | 2.229 | | 40.57 | | | С |
| | ATOM | 5209 | | VAL A 332 | | 24.912 | 5.525 | 3.187 | | 39.73 | | | С |
| 20 | ATOM | 5211 | | VAL A 332 | | 25.881 | | 1.612 | 1.00 | 41.22 | | | С |
| 30 | MOTA | 5215 | CG2 | VAL A 332 | | 22.424 | 5.582 | 1.853 | | 42.39 | | | С |
| | MOTA | 5219 | 0 | VAL A 332 | | 21.729 | 6.293 | 2.599 | | 41.60 | | | 0. |
| | ATOM | 5220 | N | MET A 333 | | 22.203 | 4.285 | 1.594 | 1.00 | 37.82 | | | N |
| | ATOM | 5221 | | MET A 333 | | 21.117 | 3.471 | 2.170 | 1.00 | 36.93 | | | С |
| 25 | MOTA | 5223 - 5225 | CB | MET A 333 | | 20.723 | 2.317 | | 1.00 | 37.72 | | • | С |
| 35 | MOTA | 5228 | CG | MET A 333 | | 20.166 | 2.782 | -0.085 | 1.00 | 41.56 | | | С |
| | MOTA | 5231 | SD | MET A 333 | | 19.579 | 1.455 | -1.132 | 1.00 | 50,56 | | | S |
| | MOTA | 5232 | CE | MET A 333 | | 18.013 | 1.284 | -0.388 | 1.00 | 55.20 | | - | С |
| | MOTA | 5236 | C | MET A 333 | | 21.588 | 2.919 | 3.503 | 1.00 | 41.46 | | | С |
| 40 | MOTA | 5237 | ŏ | MET A 333 | | 22.205 | 1.777 | 3.611 | 1.00 | 39.46 | | | 0 |
| 40 | MOTA MOTA | 52:38 | N | GLY A 334 | | 21.291 | 3.762 | 4.508 | 1.00 | 40.49 | | | N |
| | ATOM | | CA | | | 21.812 | 3.648 | 5.846 | 1.00 | 38.05 | | | С |
| | | 5243 | C | GLY A 334 | | 20.941 | | 6.789 | 1.00 | 38.82 | | | С |
| | ATOM | 5244 | o | GLY A 334 | | 19.921 | 2.335 | 6.417 | 1.00 | 44.15 | | | 0 |
| 45 | MOTA MOTA | 5245 | N | ALA A 335 | | 21.359 | | . 8.045 | 1.00 | 38.69 | | | N |
| . 43 | | 5247 | CA | | | 20.658 | | 9.044 | 1,.00 | 38,89 | | | С |
| | ATOM | 5247 | CB | | | 21.021 | | 10.403 | 1.00 | 39.90 | | • | С |
| | MOTA | 5253 | C | | | 19.193 | | 8.825 | | 42.45 | | | C |
| | ATOM | | | ALA A 335 | | 18.353 | | 8.827 | 1.00 | 41.48 | .2 | | . 0 |
| 50 | ATOM | 5254 5255 | N | VAL A 336 | | 18.830 | | 8.611 | | 43.44 | | | N |
| 50 | MOTA | | CA | | | 17.425 | | | | 46.66 | | | C |
| | MOTA | 5257 | CB | | | 16.973 | _ | | | 49.40 | | | C |
| | ATOM | 5259 | | 1 VAL A 336 | | 17.623 | | | | 55.39 | | | С |
| | ATOM | 5261 | | 2 VAL A 336 | | 17.340 | | | | 52.52 | | | С |
| | MOTA | 5265 | | VAL A 336 | | 16.921 | | | | 46.80 | | | С |
| 55 | MOTA | 5269 | C | VAL A 336 | | 16.221 | | | | 0 48.30 | | | 0 |
| | ATOM | 5270 | 0 | ILE A 337 | | 17.318 | | | | 0 45.47 | | | N |
| | ATOM | 5271 | N | | | 16.677 | _ | | | 36.74 | | | С |
| | ATOM | 5273 | CA | | | 17.298 | _ | | | 0 39.78 | | | С |
| ~ | MOTA | 5275 | CE | 3 ILE A 337 | | 17.290 | | | | 0 36.27 | | | С |
| 60 | ATOM | 5277 | | ol ILE A 337 | | 15.779 | | | | 0 43.14 | | | С |
| | ATOM | 5280 | UL |)T TRE W 221 | | 13.775 | , 3.133 | | | · | | | |

| 5 | ATOM | 5284 | CG2 | ILE A | 337 | 16.671 | 1.450 | 2.978 | 1.00 34.84 | • | | С |
|------|------|------|-----|-------|--------|--------|---------|--------|------------|---|-----|------------|
| | MOTA | 5288 | С | ILE F | 337 | 16.885 | 0.804 | 5.806 | 1.00 39.51 | | - | С |
| | ATOM | 5289 | 0 | ILE A | 337 | 16.013 | -0.096 | 5.623 | 1.00 35.70 | | | О |
| | MOTA | 5290 | N | MET A | 338 | 18.031 | 0.511 | 6.397 | 1.00 38.60 | | | N |
| | ATOM | 5292 | CA | MET A | 338 | 18.215 | -0.928 | 6.662 | 1.00 39.01 | | | С |
| 10 | MOTA | 5294 | CB | MET A | 338 | 19.673 | -1.259 | 7.028 | 1.00 37.15 | | | С |
| | ATOM | 5297 | CG | MET A | 338 | 20.587 | -1.321 | 5.812 | 1.00 38.15 | | | С |
| | ATOM | 5300 | SD | MET I | 338 | 22.320 | -1.770 | 6.100 | 1.00 49.00 | | | S |
| | ATOM | 5301 | CE | MET A | 338 | 22.236 | -3.500 | 6.563 | 1.00 47.85 | | ٠. | С |
| | ATOM | 5305 | С | MET A | 338 | 17.197 | -1.470 | 7.680 | 1.00 36.06 | | | C |
| 15 | ATOM | 5306 | o | | 338 | 16.768 | -2.596 | 7.615 | 1.00 40.65 | • | • | 0 |
| | ATOM | 5307 | N | GLU A | | 16.780 | -0.644 | 8.610 | 1.00 43.64 | | | N |
| | ATOM | 5309 | CA | GLU A | | 15.981 | -1.092 | 9.755 | 1.00 43.34 | | | С |
| | ATOM | 5311 | СВ | GLU A | 339 | 15.922 | 0.036 | 10.811 | 1.00 44.54 | | | С |
| • | ATOM | 5314 | CG | GLU A | 339 | 16.905 | -0.101 | 11.984 | 1.00 50.03 | | | С |
| 20 | ATOM | 5317 | CD | GLU A | | 17.134 | 1.179 | 12.854 | 1.00 50.19 | | | С |
| | ATOM | 5318 | | GLU A | | 18.297 | 1.508 | 13.284 | 1.00 50.60 | | | 0 |
| | ATOM | 5319 | | GLU A | | 16.170 | 1.853 | 13.133 | 1.00 52.29 | | - ' | 0 |
| • | ATOM | 5320 | С | | A 339 | 14.593 | -1.616 | 9.375 | 1.00 44.44 | | | С |
| | ATOM | 5321 | 0 | | A 339 | 13.825 | -2.079 | 10.235 | 1.00 48.83 | | | 0 |
| 25 | ATOM | 5322 | N | | A 340 | 14.257 | -1.572 | 8.096 | 1.00 37.01 | | | N |
| | ATOM | 5324 | CA | | A 340 | 13.003 | -2.140 | 7.664 | 1.00 35.04 | | | C |
| | ATOM | 5327 | С | | A 340 | 13.074 | -3.539 | 7:035 | 1.00 37.57 | | | С |
| | ATOM | 5328 | ō | | A 340 | 12.067 | -4.268 | 6.954 | 1.00 30.82 | | | 0 |
| | MOTA | 5329 | N | | A 341 | 14.251 | -3.954 | 6.584 | 1.00 36.28 | | | N |
| 30 - | ATOM | 5331 | CA | | A 341 | 14.284 | -5.201 | 5.860 | 1.00 37.94 | | | С |
| 50 | ATOM | 5333 | CB. | | A 341 | 14.549 | -4.833 | 4.467 | 1.00 35.78 | | | С |
| | ATOM | 5336 | CG | | A 341 | 13.721 | -3.727 | 4.036 | 1.00 36.57 | | | С |
| | ATOM | 5337 | | | A 341 | 14.141 | -2.449 | 4.214 | 1.00 42.48 | | | С |
| | ATOM | 5339 | | | A 341 | 13.364 | -1.430 | 3.810 | 1.00 45.68 | | | · C |
| 35 | ATOM | 5341 | CZ | | A 341 | 12.165 | -1.691 | 3.237 | 1.00 43.50 | | | С |
| - | MOTA | 5343 | | | A 341 | 11.735 | -2.983 | 3.058 | 1.00 39.45 | | | С |
| | MOTA | 5345 | | | A 341 | 12.493 | -3.971 | 3.451 | 1.00 39.09 | | | С |
| | ATOM | 5347 | С | | A 341 | 15.287 | -6.189 | 6.323 | 1.00 37.29 | | | С |
| | ATOM | 5348 | 0 | | A 341 | 16.019 | -5.890 | 7.200 | 1.00 41.19 | | | 0 |
| 40 | ATOM | 5349 | N | | A 342 | 15.294 | -7.383 | 5.745 | 1.00 38.28 | • | | N |
| | ATOM | 5351 | CA | | A 342 | | -8.381 | 6.079 | 1.00 39.65 | | • | С |
| | ATOM | 5353 | CB | TYR : | A 342 | 15.710 | -9.774 | 6.073 | 1.00 40.40 | | | · C |
| | ATOM | 5356 | CG | | A 342 | | -10.890 | 6.407 | 1.00 41.95 | | | С |
| | ATOM | 5357 | CD1 | TYR . | A 342 | 17.625 | -10.727 | 7.340 | 1.00 43.94 | | | С |
| 45 | MOTA | 5359 | CE1 | TYR . | A 342 | 18.488 | -11.731 | 7.651 | 1.00 48.72 | | | . C |
| | ATOM | 5361 | CZ | | A 342 | | -12.947 | 7.036 | 1.00 49.33 | | | С |
| | ATOM | 5362 | ОН | | A 342 | | -13.922 | 7.408 | 1.00 51.44 | | | 0 |
| | ATOM | 5364 | CE2 | TYR . | A 342 | 17.442 | -13.159 | 6.091 | 1.00 43.68 | | | , C |
| | ATOM | 5366 | | | A 342 | | -12.122 | 5.784 | 1.00 47.27 | | | С |
| 50 | ATOM | 5368 | С | | A 342 | | -8.182 | 4.875 | 1.00 36.83 | | | С |
| | ATOM | 5369 | 0 | | A 342 | | -8.334 | 3.816 | 1.00 38.58 | | | 0 |
| | ATOM | 5370 | N | | A 343 | | -7.818 | 4.992 | 1,00 32.01 | | | N |
| ٠ | ATOM | 5372 | CA | | A 343 | | -7.554 | 3.788 | 1.00 31.56 | | | С |
| | ATOM | 5374 | СВ | | A 343 | , | -6.367 | 3.980 | 1.00 35.24 | | • | С |
| 55 | ATOM | 5376 | | | A 343 | | -5.970 | 2.673 | 1.00 32.39 | | • | С |
| 75 | ATOM | 5380 | | | A 343 | | -5.211 | 4.529 | 1.00 41.31 | | | С |
| | ATOM | 5384 | C. | | A 343 | | -8.701 | 3.611 | 1.00 29.86 | | | С |
| | ATOM | 5385 | Ö | | A 343 | | | 4.562 | 1.00 31.04 | | | 0 |
| | MOTA | 5386 | N | | A 344 | | | | 1.00 33.91 | | | N |
| 60 | ATOM | 5388 | CA | | A 344 | | -10.337 | 2.216 | 1.00 28.64 | | | C |
| UU | ATOM | 5390 | CB | | A 344 | | -11.348 | 1.500 | 1.00 23.00 | | | C |
| | MION | 3330 | CD | A VID | ., Ja4 | 20.120 | 11.540 | 2.500 | 1.00 00.00 | | | • |

| _ | | E202 | CC1 | VAL A 344 | 21.253 -12.622 1.272 1.00 39 | .15 C | |
|-------------|------|----------------|----------|------------------------|---|---------|----------|
| 5 | ATOM | 5392 5396 - | CGI | VAL A 344 | 19.173 -11.671 2.320 1.00 32 | .27 C | |
| | ATOM | | CGZ | VAL A 344 | 22.433 -10.004 1.360 1.00 32 | .31 C | |
| | MOTA | 5400 | 0 | VAL A 344 | 22.298 -9.878 0.166 1.00 36 | .99 0 | |
| | ATOM | 5401 | | PHE A 345 | 23.621 -9.871 1.945 1.00 36 | _ | |
| 10 | ATOM | 5402 | N | PHE A 345 | 24.822 -9.592 1.141 1.00 36 | .18 C | |
| 10 | ATOM | 5404 | CA | PHE A 345 | 25.861 -8.841 1.954 1.00 38 | | |
| | MOTA | 5406 | CB | PHE A 345 | 25.449 -7.408 2.249 1.00 37 | _ | |
| | ATOM | 5409 | CG | | 25.889 -6.348 1.501 1.00 42 | | |
| | ATOM | 5410 | | PHE A 345 | 25.487 -5.139 1.797 1.00 40 | _ | |
| | MOTA | 5412 | | PHE A 345 PHE A 345 | 24.621 -4.914 2.850 1.00 36 | | |
| 15 | ATOM | 5414 | CZ | | 24.186 -5.924 3.581 1.00 34 | | |
| | ATOM | 5416 | | PHE A 345 | 24.597 -7.177 3.279 1.00 32 | | |
| | MOTA | 5418 | | PHE A 345 | 25.443 -10.824 0.522 1.00 36 | | |
| | ATOM | 5420 | C · | PHE A 345 | 26.486 -11.317 0.958 1.00 39 | | |
| | ATOM | 5421 | 0 | PHE A 345 | 24.785 -11.298 -0.525 1.00 3 | | |
| 20 | MOTA | 5422 | N | ASP A 346 | 25.157 -12.498 -1.257 1.00 33 | _ | |
| | MOTA | 5424 | CA | ASP A 346 | 23.865 -12.940 -1.938 1.00 4 | | |
| | MOTA | 5426 | CB | ASP A 346 | 23.993 -14.184 -2.742 1.00 4 | | |
| | ATOM | 5429 | CG | ASP A 346 | 25.122 -14.682 -2.972 1.00 4 | | |
| | MOTA | 5430 | | ASP A 346 | 22.961 -14.707 -3.196 1.00 4 | | |
| 25 | MOTA | 5431 | | ASP A 346 | 26.310 -12.270 -2.247 1.00 3 | | |
| | MOTA | 5432 | С | ASP A 346 | 26.156 -12.107 -3.481 1.00 3 | | |
| | MOTA | 5433 | 0 | ASP A 346 | 27.498 -12.256 -1.659 1.00 4 | | |
| | MOTA | 5434 | N | ARG A 347 | 28.764 -12.187 -2.385 1.00 3 | • • • • | |
| | MOTA | 5436 | CA | ARG A 347 | 29.896 -12.280 -1.348 1.00 4 | _ | |
| 30 | MOTA | 5438 | CB | | 29.903 -11.047 -0.457 1.00 3 | | |
| | ATOM | 5441 | CG | ARG A 347 | 30.720 -11.142 0.739 1.00 3 | | |
| | ATOM | 5444 | CD | ARG A 347 | | | |
| | MOTA | 5447 | NE | ARG A 347 | 32.086 -11.477 | | |
| | MOTA | 5449 | CZ | ARG A 347 | 33.029 -9.658 1.397 1.00 5 | • • • • | |
| 35 | 1110 | 5450 | | ARG A 347 | 34.372 -11.171 0.317 1.00 4 | | |
| | ATOM | 5453 | | 2 ARG A 347 | 28.920 -13.265 -3.429 1.00 3 | | |
| | MOTA | 5456 | C | ARG A 347 | 29.227 -12.993 -4.573 1.00 4 | | |
| | MOTA | 5457 | 0 | ARG A 347 | 28.699 -14.501 -3.041 1.00 4 | | |
| 40 | MOTA | 5458 | N | ALA A 348 | 28.835 -15.651 -3.960 1.00 4 | | |
| 40 | MOTA | 5460 | ·CA | ALA A 348 | 28.168 -16.883 -3.369 1.00 4 | | |
| | ATOM | 5462 | CB | ALA A 348 | 28.256 -15.440 -5.301 1.00 4 | | |
| | MOTA | 5466 | C | ALA A 348 ALA A 348 | 28.804 -15.893 -6.279 1.00 5 | | ٠ |
| | MOTA | 5467 | 0 | ARG A 349 | 27.114 -14.772 -5.347 1.00 5 | | |
| 45 | MOTA | 5468 | N | ARG A 349 | 26.435 -14.531 -6.606 1.00 4 | 5.15 C | |
| 45 . | MOTA | 5470 | CA CB | ARG A 349 | 25.008 -15.048 -6.522 1.00 4 | 6.17 C | |
| | MOTA | 5472 | CG | ARG A 349 | 25.021 -16.582 -6.566 1.00 5 | 0.92 C | |
| | ATOM | 5475 | CD | | 23.678 -17.332 -6.431 1.00 5 | | |
| | ATOM | 5478 | | ARG A 349 | 22.731 -17.167 -7.546 1.00 5 | | |
| | MOTA | 5481 | NE C7 | ARG A 349 | 21.525 -17.757 -7.576 1.00 5 | | , |
| 50 | MOTA | 5483 | CZ | | 21.140 -18.544 -6.575 1.00 5 | | |
| | ATOM | 5484 | | 1 ARG A 349 | 20.699 -17.576 -8.596 1.00 9 | | j |
| | ATOM | 5487 | , | 2 ARG A 349 | 26.515 -13.088 -7.031 1.00 | | <u>'</u> |
| | ATOM | 5490 | C | ARG A 349 | 26.054 -12.752 -8.115 1.00 | |) |
| | MOTA | 5491 | 0 | ARG A 349 | 27.108 -12.227 -6.198 1.00 | · | |
| 55 | ATOM | 5492 | N | LYS A 350 | 27.108 -12.227 | | |
| | ATOM | 5494 | CA | | 27.981 -10.696 -7.901 1.00 | _ | |
| | ATOM | 5496 | | | 28.391 -9.252 -8.257 1.00 | | |
| | MOTA | 5499 | | | | | |
| | ATOM | 5502 | | | | = = | |
| 60 | ATOM | 5505 | | | 29.595 -7.616 -9.867 1.00 30.583 -7.261 -10.973 1.00 | | |
| | MOTA | 5508 | NZ | LYS A 350 | 70.707 1.201 10.3.0 1.00 | | |

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25.878 -10.169
                                                                1.00 42.26
                                                        -6.591
                       LYS A 350
    MOTA
            5512
                                                                1.00 36.83
                                                        -7.620
                       LYS A 350 ...
                                       25.434 -9.629
    MOTA
            5513
                  0
                                                                1.00 43.25
                                                        -5.431
                                       25.198 -10.229
                       ARG A 351
            5514
    ATOM
                  N
                                                                1.00 39.90
                                                        -5.285
                       ARG A 351
                                       23.853 -9.649
            5516
                  CA
    MOTA
                                                        -5.867
                                                                1.00 38.47
                       ARG A 351
                                       22.823 -10.612
            5518
                  CB
    ATOM
                                      22.635 -11.942
                                                                1.00 40.60
                                                        -5.173
                       ARG A 351
10
    ATOM
            5521
                   CG
                                                                                      С
                                                        -6.063
                                                                1.00 43.93
                                       21.811 -12.900
                       ARG A 351
                   CD
     ATOM
            5524
                                                                                      N
                       ARG A 351
                                       21.546 -14.178
                                                        -5.418
                                                                1.00 50.64
     MOTA
            5527
                   NE
                                                                                      C
                                                                1.00 44.16
                                       20.398 -14.872
                                                        -5.490
                       ARG A 351
                   CZ
     MOTA
            5529
                                                                1.00 30.21
                                                                                      N
                                       19.376.-14.454
                                                        -6.184
                      ARG A 351
            5530
                   NH1
     MOTA
                                       20.298 -16.009
                                                        -4.839
                                                                1.00 45.65
                                                                                      N
                   NH2 ARG A 351
15
            5533
    MOTA
                                                        -3.872
                                                                1.00 34.43
                                                                                      С
                       ARG A 351
                                       23.449
                                               -9.270
            5536
                   C.
     MOTA
                                               -9.841
                                                                1.00 40.67
                                                                                      0
                                                        -2.946
            5537
                   0
                       ARG A 351
                                       23.928
     MOTA
                                               -8.292
                                                                1.00 34.43
                                                                                      N
                                                        -3.711
                       ILE A 352
                                       22.562
     MOTA
             5538
                   N
                                               -7.958
                                                                                      С
                                       21.995
                                                        -2.397
                                                                1.00 28.97
                       ILE A 352
     MOTA
             5540
                   CA
                                                                                      C
                                               -6.539
                                                                1.00 30.73
                       ILE A 352
                                                        -2.051
                                       22.232
                   CB
20
     MOTA
            .5542
                                                                1.00 31.97
                                                                                     . C
                   CG1 ILE A 352
                                               -6.288
                                                        -2.019
                                       23.729
             5544
     MOTA
                                                                1.00 34.88
                                                        -2.366
                                                                                      C
                   CD1 ILE A 352
                                       24.027
                                               -4.969
             5547
     MOTA
                                                                                      С
                                                                1.00 32.36
                       ILE A 352
                                       21.688
                                               -6.255
                                                        -0.674
             5551
                   CG2
     MOTA
                                                                                      С
                                                        -2.397
                                                                1.00 31.19
                                               -8.181
     ATOM
             5555
                   C
                       ILE A 352
                                       20.527
                                                                1.00 31.73
                                                                                      0
                                               -7.740
                                                        -3.309
                       ILE A 352
                                       19.848
25
     MOTA
             5556
                   0
                                                                                      N
                                               -8.875
                                                        -1.372
                                                                1.00 36.35
                       GLY A 353
                                       20.032
             5557
                   N
     ATOM
                                                                                       С
                                                                1.00 37.89
                       GLY A 353
                                               -9.239
                                                        -1.311
                                       18.629
     ATOM
             5559
                   CA
                                                                1.00 38.37
                                                                                       С
                       GLY A 353
                                               -8.451
                                                        -0.291
                                       17.850
             5562
                   С
     ATOM
                                                                1.00 42.00
                                                         0.759
                                                                                       0
                                       18.393
                                               -8.137
                       GLY A 353
                   0
     MOTA
             5563
                                                                1.00 37.07
                      PHE A 354
                                       16.586
                                               -8.143
                                                        -0.592
30
                   Ν.
     MOTA
             5564
                                                         0.352
                                                                1.00 31.53
                                               -7.427
             5566
                   CA
                       PHE A 354
                                       15.730
     MOTA
                                                                1.00 29.79
                                                -5.999
                                                        -0.164
                                       15.379
                       PHE A 354
     MOTA
             5568
                   CB
                                                                                       C
                                       16.557
                                                -5.063
                                                        -0.308
                                                                1.00 26.28
                       PHE A 354
     ATOM
             5571
                   CG
                                                                                       С
                                                                1.00 32.33
                                                -5.078
                                                        -1.450
                   CD1 PHE A 354
                                       17.323
             5572
     MOTA
                                                        -1.598
                                                                1.00 34.84
                                       18.424
                                                -4.209
                   CE1 PHE A 354
35
     ATOM
             5574
                                               -3.320
                                                        -0.581
                                                                1.00 35.73
                       PHE A 354
                                       18.742
             5576
                   CZ
     MOTA
                                                                                       С
                                                -3.287
                                                         0.571
                                                                1.00 27.61
                   CE2 PHE A 354
                                       17.971
     ATOM
             5578
                                                                                       С
                                                         0.704
                                                                1.00 28.09
                                                -4.148
                   CD2 PHE A 354
                                       16.885
     MOTA
             5580
                                                                                       С
                       PHE A 354
                                       14.415
                                                         0.649
                                                                 1.00 31.75
                                                -8.191
     MOTA
             5582
                   С
                                                                                       0
                                       13.752
                                                        -0.273
                                                                1.00 35.59
                       PHE A 354
                                                -8.665
40
             5583
                   0
     ATOM
                                                                 1.00 26.00
                                                                                       N
                                                         1.934
                                       14.065
                                                -8.308
             5584
                   N
                       ALA A 355
     MOTA
                                                                 1.00 25.47
                                                         2.345
                       ALA A 355
                                       12.707
                                                -8.676
             5586
                   CA
     MOTA
                                       12.652 -10.035
                                                         2.579
                                                                 1.00 28.36
             5588
                       ALA A 355
     MOTA
                   CB
                                                                 1.00 30.38
                                               -7.961
                                                         3.602
                       ALA A 355
                                       12.222
     ATOM
             5592
                   С
                                                -7.387
                                                         4.333
                                                                 1.00 31.09
                       ALA A 355
                                       13.009
45
     MOTA
             5593
                   0
                                                -7.991
                                                         3.860
                                                                 1.00 35.80
                       VAL A 356
                                       10.912
             5594
                   N
     MOTA
                                                                 1.00 37.43
                                                                                       C
                                                         4.958
                       VAL A 356
                                       10.326
                                                -7.206
             5596
                   CA
     MOTA
                                                -7.269
                                                                 1.00 36.49
                                                         4.990
             5598
                       VAL A 356
                                        8.800
     MOTA
                   CB
                                                         5.891
                                                                 1.00 41.38
                                                                                       С
                   CG1 VAL A 356
                                        8.258
                                                -6.199
             5600
     MOTA
                                                -7.092
                                                         .3.695
                                                                1.00 35.72
50
     MOTA
                       VAL A 356
                                        8.253
             5604
                   CG2
                                                                                       C
                                                -7.852
                                                          6.243
                                                                1.00 41.52
                                        10.735
      MOTA
             5608
                   С
                        VAL A 356
                                                          6.331
                                                                 1.00 37.93
                                                                                       0
                                                -9.066
                        VAL A 356
             5609
                                        10.683
      ATOM
                   0
                                                          7.242
                                                                 1.00 43.38
                                                                                       N
                        SER A 357
                                      11.104
                                                -7.051
      ATOM
             5610
                   N
                                                                                       C
                        SER A 357
                                        11.551
                                                -7.584
                                                          8.506
                                                                 1.00 39.52
      MOTA
             5612
                   CA
                                                                                       C
                        SER A 357
                                                -6.514
                                                          9.235
                                                                 1.00 45.00
                                        12.327
 55
      MOTA
             5614
                   CB
                                                                                       0
                                                -7.090
                                                         10.258
                                                                 1.00 55.64
                        SER A 357
                                        13.156
             5617
                   OG
      MOTA
                                                          9.368
                                                                 1.00 45.19
                        SER A 357
                                        10.410
                                                -8.000
             5619
                   С
      MOTA
                                                                 1.00 52.71
                                                          9.314
             5620
                   0
                        SER A 357
                                        9.356
                                                -7.417
      MOTA
                                                -9.023
                                                         10.193
                                                                 1.00 51.62
                        ALA A 358
                                        10.599
      ATOM
             5621
                   N
                                                -9.402
                                                         11.143
                                                                 1.00 47.19
                                       9.558
                        ALA A 358
 60
      MOTA
             5623
                    CA
                                         9.455 -10.874
                                                         11.270
                                                                 1.00 44.33
                        ALA A 358
      MOTA
             5625
                    CB
```

| | | | | | | | | | | • | | | |
|------------|------|--------------|----------|-------------|---|--------|--------|--------|------|---------|---|----------|--------------|
| 5 | ATOM | 5629 | C. | ALA A 358 | | 9.858 | -8.814 | 12.486 | | 53.26 | | | C |
| . • | MOTA | 5630 | 0 | ALA A 358 | | 9.324 | -9.302 | 13.472 | | 58.72 | | | 0 |
| | | 5631 | N | CYS A 359 | • | 10.720 | -7.790 | 12.540 | | 54.45 | | | N |
| | MOTA | 5633 | CA | CYS A 359 | | 10.962 | -7.065 | 13.779 | | 52.85 | | | C |
| | ATOM | 5635 | CB | CYS A 359 | | 12.325 | -7.455 | 14.429 | | 55.72 | | | С |
| 10 | ATOM | 5638 | SG | CYS A 359 | | 13.911 | -6.785 | 13.755 | | 65.10 | | | S |
| 10 | ATOM | 5639 | C | CYS A 359 | | 10.793 | -5.543 | 13.583 | | 53.76 | | | С |
| | ATOM | 5640 | ō | CYS A 359 | | 11.047 | -4.789 | 14.519 | | 60.53 | | | 0 |
| | MOTA | 5641 | N | HIS A 360 | | 10.332 | -5.075 | 12.412 | | 45.54 | | | N |
| | ATOM | 5643 | CA | HIS A 360 | | 10.265 | -3.631 | 12.161 | | 38.19 | | | С |
| 15 | ATOM | 5645 | CB | HIS A 360 | | 10.274 | -3.291 | 10.655 | | 31.06 | | | С |
| 15 | ATOM | 5648 | CG | HIS A 360 | | | -3.409 | 9.972 | 1.00 | 34.23 | | \ | С |
| | ATOM | 5649 | | HIS A 360 | | 8.422 | -4.617 | 9.566 | 1.00 | 43.85 | | | N |
| | ATOM | 5.651 | | HIS A 360 | | 7.259 | -4.425 | 8.979 | 1.00 | 30.40 | | | С |
| - | ATOM | 5653 | | HIS A 360 | | 7.010 | -3.130 | 8.992 | 1.00 | 36.44 | | | N |
| 20 | | 5655 | | HIS A 360 | | 8.051 | -2.475 | 9.607 | 1.00 | 29.91 | | | С |
| 20 | ATOM | | C | HIS A 360 | | 9.170 | -2.820 | 12.921 | 1.00 | 41.87 | | | \mathbf{C} |
| | ATOM | 5657 | | HIS A 360 | | 8.085 | -3.281 | 13.248 | | 47.13 | | | 0 |
| | ATOM | 5658 | 0 | VAL A 361 | | 9.488 | -1.576 | 13.194 | | 36.30 | | | N |
| | MOTA | 5659 | N | VAL A 361 | | 8.626 | -0.768 | 13.971 | | 36.06 | | | С |
| ٥ċ | ATOM | 5661 | CA | | | 9.448 | 0.396 | 14.601 | | 33.69 | , | | С |
| 25 | ATOM | 5663 | CB | VAL A 361 | | 8.519 | 1.388 | 15.203 | | 33.28 | | | С |
| | ATOM | 5665 | | VAL A 361 | | 10.371 | -0.136 | 15.590 | | 30.28 | | | С |
| | ATOM | 5669 | | VAL A 361 | | 7.498 | -0.219 | 13.100 | | 35.37 | | | Ç |
| | MOTA | - 5673 | C | VAL A 361 | | 7.749 | 0.397 | 12.095 | | 28.73 | | | Ó |
| | MOTA | 5674 | 0 | VAL A 361 | | | -0.453 | 13.489 | | 38.93 | | | N |
| 30 | MOTA | 5675 | N | HIS A 362 | | 6.262 | | 12.726 | | 43.25 | | | C |
| | MOTA | 5677 | CA | HIS A 362 | | 5.119 | | 11.462 | | 43.67 | • | | Ċ |
| | MOTA | 5679 | CB | HIS A 362 | | 4.939 | -0.771 | 11.705 | | 46.38 | | | č |
| • | ATOM | 5682 | CG | HIS A 362 | | 4.555 | -2.203 | 11.703 | | 49.03 | | | N |
| | ATOM | 5683 | | HIS A 362 | • | 5.479 | -3.210 | 12.037 | | 50.56 | • | | C |
| 35 | ATOM | 5685 | | HIS A 362 | | 4.855 | -4.363 | | | 45.23 | | | N |
| | MOTA | 5687 | | 2 HIS A 362 | | 3.558 | -4.143 | 12.013 | | 51.21 | | | c |
| | MOTA | 5689 | CD2 | 2 HIS A 362 | | 3.345 | -2.799 | 11.810 | | 44.78 | | | č |
| | MOTA | 5691 | С | HIS A 362 | | 3.831 | 0.124 | 13.587 | | 49.93 | | | ő |
| | MOTA | 5692 | О | HIS A 362 | | 3.871 | -0.147 | 14.749 | | 48.91 | | | N |
| 40 | MOTA | 5693 | N | ASP A 363 | | 2.704 | 0.524 | 13.028 | | 48.51 | | | C |
| | MOTA | 5695 | ÇA | ASP A 363 | | 1.412 | | 13.729 | | | | | č |
| | MOTA | 5697 | CB | ASP A 363 | | 0.779 | 1.835 | 13.601 | | 48.80 | | | c |
| • | MOTA | 5700 | CG | ASP A 363 | | 0.798 | 2.252 | 12.190 | | 56.05 | | | o |
| ٠ | MOTA | 5701 | | 1 ASP A 363 | | 0.064 | 1.570 | 11.427 | | 62.04 | | | 0 |
| 45 | MOTA | 5702 | OD: | 2 ASP A 363 | | 1.530 | 3.170 | 11.732 | | 53.10 | | | C |
| | ATOM | 5703 | С | ASP A 363 | | 0.583 | -0.390 | 12.839 | | 50.55 | | | |
| | ATOM | 5704 | 0 | ASP A 363 | | 1.082 | -0.877 | 11.824 | | 49.82 | | | 0 |
| | ATOM | 5705 | N | GLU A 364 | | -0.698 | | | | 51.52 | | | N |
| | ATOM | 5707 | CA | | | -1.506 | -1.526 | 12.443 | 1.00 | 50.07 | | | С |
| 50 | ATOM | 5709 | СВ | • | | -2.705 | -1.964 | 13.242 | | 54.11 | | | С |
| 50 | ATOM | 5712 | CG | | | -3.727 | -0.871 | 13.464 | 1.00 | 56.03 | | | С |
| | ATOM | 5715 | CD | | | -5.070 | -1.412 | 13.986 | | 64.46 | | | .C |
| | ATOM | 5716 | | 1 GLU A 364 | | -6.040 | | 13.967 | 1.00 | 76.03 | | | 0 |
| | MOTA | 5717 | | 2 GLU A 364 | | -5.182 | | 14.399 | 1.00 | 0 46.64 | | | 0 |
| 55 | | 5718 | C | GLU A 364 | | -1.989 | | | | 47.66 | | | С |
|)) | ATOM | 5719 | ő | GLU A 364 | | -2.524 | | | | 0 47.48 | • | | . 0 |
| | MOTA | | | PHE A 365 | | -1.799 | | | | 0 41.55 | | | N |
| | MOTA | 5720 5722 | N | | | -2.309 | | | | 0 44.15 | | | . C |
| | MOTA | | CA CB | | | -2.603 | | | | 0 42.84 | | | С |
| <i>(</i> 0 | MOTA | 5724 | | | | -3.640 | | | | 0 42.11 | | | С |
| 60 | ATOM | 5727 | | | | -3.391 | | | | 0 43.74 | | | С |
| | MOTA | 5728 | CD | 1 PHE A 365 | , | 3.331 | 3.047 | 24.120 | | | | | |

| 5 | ATOM | 5730 | CE1 | PHE F | A 365 | | -4.332 | 3.195 | 13.033 | 1.00 43.17 | | | С |
|-----|---------------|---------------|-----|-------|--------|---|--------|--------|----------------|--------------------------|----|---|----|
| • | ATOM | 5732 | CZ | PHE A | A 365 | | -5.532 | 2.685 | 12.820 | 1.00 47.95 | | | С |
| | MOTA | 5734 | CE2 | PHE F | A 365 | | -5.793 | 2.006 | 11.673 | 1.00 50.59 | | | С |
| | ATOM | 5736 | CD2 | PHE A | A 365 | | -4.869 | 1.858 | 10.771 | 1.00 47.37 | | | С |
| | MOTA | 5738 | C | PHE A | A 365 | | -1.462 | 0.662 | 8.321 | 1,00 46.25 | | | C |
| 10 | ATOM | 5739 | Ō | | A 365 | | -2.031 | 0.487 | 7.227 | 1.00 49.35 | | | 0 |
| | ATOM | 5740 | N | | A 366 | | -0.143 | 0.745 | 8.428 | 1.00 42.85 | | | N |
| | ATOM | 5742 | CA | | A 366 | | 0.796 | 0.645 | 7.309 | 1.00 41.91 | | | С |
| | MOTA | 5744 | СВ | | A 366 | | 1.398 | 1.997 | 6.985 | 1.00 40.96 | | | С |
| | MOTA | 5747 | CG | | A 366 | | 0.536 | 2.993 | 6.424 | 1.00 40.90 | | | С |
| 15 | ATOM | 5750 | CD. | | A 366 | | 1.341 | 4.073 | 5.811 | 1.00 40.88 | | | С |
| ,13 | ATOM | 5753 | NE | | A 366 | | 1.839 | 4.979 | 6.843 | 1.00 40.97 | • | • | N |
| | ATOM | 5755 | CZ | | A 366 | | 1.893 | 6.275 | 6.661 | 1.00 40.91 | | | С |
| | ATOM | 5756 | | | A 366 | | 1.476 | 6.743 | 5.493 | 1.00 36.36 | | | N |
| | ATOM | 5759 | | | A 366 | | 2.346 | 7.096 | 7.609 | 1.00 40.33 | | , | N |
| 20 | ATOM | 5762 | C | | A 366 | | 2.061 | -0.090 | 7.758 | 1.00 41.93 | | | C |
| 20. | | | | | A 366 | | 2.491 | 0.129 | 8.894 | 1.00 41.59 | | | ō |
| | ATOM | 5763. 5764 | N | | A 367 | | 2.677 | -0.865 | 6.847 | 1.00 37.72 | | | N |
| | MOTA | 5766 | CA | | A 367 | | 3.839 | -1.681 | 7.138 | 1.00 33.65 | | • | C |
| | ATOM | | | | A 367 | | 3.469 | -3.107 | 7.143 | 1.00 42.32 | | | Ċ |
| 25 | MOTA | 5768 | CB | | A 367 | | 4.646 | -3.854 | 6.891 | 1.00 43.84 | | | ő |
| 25 | ATOM | 5770 | | | | | 2.528 | -3.460 | 5.969 | 1.00 43.37 | | | Č |
| | ATOM | 5772 | CG2 | | A 367 | | | -1.507 | 6.066 | 1.00 43.37 | | | č |
| • | MOTA | 5776 | С | | A 367 | | | | | 1.00 32.72 | | • | Ö |
| | MOTA | 5777 | 0 | | A 367 | | | -1.157 | 4.970 6.359 | 1.00 34.38 | | | N |
| 20 | ATOM | 5778 | N | | A 368 | | 6.110 | -1.702 | | 1.00 39.92 | | | C |
| 30 | ATOM | 5780 | CA | | A 368 | | 7.135 | -1.504 | 5.307 | | | | c |
| | MOTA | 5782 | CB | | A 368 | | 8.485 | -1.608 | 5.870 | 1.00 38.72 | | | C |
| | ATOM | 5786 | C | | A 368 | | 6.910 | -2.529 | 4.180 | 1.00 43.33 | | | Ö |
| | ATOM | 5787 | 0 | | A 368 | | 6.181 | -3.498 | 4.382 | 1.00 47.27 | | | N |
| 25 | ATOM | 5788 | N | | A 369 | | 7.494 | -2.369 | 2.998 | 1.00 41.85 | | | C |
| 35 | ATOM | 5790 | CA | | A 369 | | 7.115 | -3.346 | 1.966 | 1.00 38.56 | | | C |
| | ATOM | 5792 | CB | | A 369 | | 5.832 | -2.891 | 1.277 | 1.00 40.40 | | | c |
| | MOTA | 5796 | C | | A 369 | | 8.162 | -3.635 | 0.928 | 1.00 29.85 1.00 36.35 | | | o |
| | MOTA | 5797 | 0 | | A 369 | | 9.095 | -2.854 | | 1.00 36.33 | | | N. |
| 40 | MOTA | 5798 | N | | A 370 | | 7.966 | -4.769 | 0.274 | | | | C |
| 40 | MOTA | 5800 | CA | | A 370 | | 8.831 | -5.260 | -0.769 | 1.00 29.57 | | | Ç |
| | MOTA | 5802 | CB | | A 370 | | 9.849 | -6.185 | -0.229 | 1.00 26.20 | | | Ċ |
| | ATOM | 5804 | | | A 370 | | 10.757 | -6.632 | -1.321 | 1.00 32.44 | | | c |
| | MOTA | 5808 | | | A 370 | | 10.689 | -5.482 | 0.827 | 1.00 30.95 | | | c |
| 4 | ATOM | 5812 | С | | A 370 | | 7.929 | -5.941 | -1.796 | 1.00 31.92 | | | 0 |
| 45 | MOTA | 5813 | 0 | | A 370 | | 7.225 | | -1.490 | 1.00 36.53 | | | N |
| | ATOM | 5814 | N | | A 371 | | 7.945 | -5.452 | -3.029 | 1.00 33.29 | | | C |
| | MOTA | 5816 | CA | | A 371 | | 6.979 | -5.876 | -3.989 | 1.00 28.61 | | | C |
| | MOTA | 5818 | СВ | | A 371 | | | -4.939 | | 1.00 32.04 | • | | |
| | ATOM | 5821 | CG | | A 371 | • | 5.266 | -4.723 | -2.470 | 1.00 38.80 | | • | C |
| 50 | MOTA | 5824 | CD | | A 371 | | 4.374 | -3.505 | | 1.00 44.41 | ٠. | | С |
| | MOTA | 5825 | | | A 371 | | 3.119 | -3.685 | -2.230 | 1.00 55.91 | | | 0 |
| | ATOM | 5826 | | | A 371 | | 4.919 | -2.370 | | 1.00 45.34 | | | 0 |
| | ATOM | 5827 | ·C | | A. 371 | | 7.625 | -5.792 | -5.338 | 1.00 34.43 | | | C |
| | MOTA | 5828 | . 0 | | A 371 | | 8.335 | -4.857 | -5.587 | 1.00 31.86 | | | 0 |
| 55 | MOTA | 5829 | N | | A 372 | | 7.410 | -6.797 | -6.201 | 1.00 41.45 | | | N |
| | MOTA | 5831 | CA | GLY | A 372 | | 7.862 | -6.730 | -7.585 | 1.00 44.38 | | | C |
| | MOTA | 5834 | С | GLY . | A 372 | | 7.151 | -7.793 | -8.402 | 1.00 49.60 | | | C |
| | MOTA | 5835 | 0 | GLY . | A 372 | | 6.383 | -8.580 | | 1.00 48.56 | | | 0 |
| | MOTA | 5836 | N | PRO | A 373 | | 7.383 | -7.862 | | 1.00 50.59 | | | N |
| 60 | MOTA | 5837 | CA | PRO | A 373 | | 8.248 | | -10.495 | 1.00 49.61 | | | С |
| | ATOM | 5839 | CB | PRO | A 373 | | 8.726 | -7.915 | -11.588 | 1.00 51.13 | | | C |
| | • . • • • • • | | | | | | | | | | | | |

| 5 ATOM 5845 CG PRO A 373 6.799 -8.918 -10.531 1.00 50.00 ATOM 5848 C PRO A 373 6.799 -8.918 -10.531 1.00 50.00 ATOM 5849 C PRO A 373 6.324 -6.033 -11.428 1.00 59.43 ATOM 5849 C PRO A 373 6.324 -6.033 -11.428 1.00 59.43 ATOM 5852 CA PRE A 374 7.576 -3.700 -12.360 1.00 55.44 ATOM 5852 CA PRE A 374 7.576 -3.700 -12.360 1.00 55.44 ATOM 5854 CB PRE A 374 7.579 -2.369 -11.615 1.00 53.98 ATOM 5857 CB PRE A 374 7.679 -2.369 -10.227 1.00 51.03 ATOM 5858 CD1 PRE A 374 7.999 -2.369 -10.227 1.00 51.03 ATOM 5858 CD1 PRE A 374 7.999 -2.743 -9.179 1.00 47.22 ATOM 5866 CC2 PRE A 374 7.676 -7.895 1.00 52.78 ATOM 5866 CC2 PRE A 374 5.860 -2.083 -8.737 1.00 49.61 ATOM 5866 CP PRE A 374 5.860 -2.083 -8.737 1.00 49.61 ATOM 5867 CP PRE A 374 5.860 -2.083 -8.737 1.00 49.61 ATOM 5869 OPER A 374 9.536 -3.729 -13.651 1.00 59.75 ATOM 5867 CR VAL A 375 8.460 -2.063 -9.987 1.00 49.61 ATOM 5872 CA VAL A 375 8.460 -3.007 -16.020 1.00 72.14 ATOM 5880 CC2 VAL A 375 8.601 -3.444 -18.453 1.00 73.03 ATOM 5880 CC2 VAL A 375 8.601 -3.444 -18.453 1.00 73.03 ATOM 5880 CC2 VAL A 375 8.601 -3.444 -18.453 1.00 73.03 ATOM 5880 CC2 VAL A 375 8.601 -3.444 -18.453 1.00 71.54 ATOM 5880 CC3 VAL A 375 8.601 -3.444 -18.453 1.00 71.54 ATOM 5880 CC3 VAL A 375 8.601 -3.444 -18.453 1.00 71.54 ATOM 5880 CC3 VAL A 375 8.601 -3.444 -18.453 1.00 71.54 ATOM 5880 CC3 VAL A 375 8.751 -1.541 -16.347 1.00 76.96 ATOM 5880 CC3 VAL A 375 8.751 -1.541 -16.347 1.00 76.96 ATOM 5890 CB TRR A 376 11.055 0.740 -14.4901 1.00 89.17 ATOM 5890 CB TRR A 376 11.055 0.740 -14.4901 1.00 89.17 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.23 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.73 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.70 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.70 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.70 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.70 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.70 ATOM 5890 CB TRR A 376 11.550 0.063 -1.7389 1.00 88.70 ATOM 5990 CD TRR A 378 1.00 4.00 0.00 0.00 0.00 0.00 0.00 0.00 | _ | | | | × 272 | | 7.732 | -9.025 -11.666 | 1.00 50.04 | | | C . |
|--|------------|------|------|------|------------|---|--------|----------------|--------------|---|---|------------|
| ATOM 5648 C PRO A 373 | 5 | MOTA | | | PRO A 373 | - | | | 1.00 50.00 | | | С |
| ATOM 5849 O PRO A 373 | | MOTA | 5845 | | | | | | | | | C |
| ATOM 5850 N PHE A 374 7.576 -3.700 -12.360 1.00 55.44 ATOM 5852 CA PHE A 374 7.576 -3.700 -12.360 1.00 55.44 ATOM 5854 CB PHE A 374 7.579 -2.369 -11.615 1.00 53.01 ATOM 5856 CD PHE A 374 7.163 -2.396 -10.227 1.00 51.03 ATOM 5856 CD PHE A 374 7.163 -2.396 -10.227 1.00 51.03 ATOM 5856 CD PHE A 374 7.448 -2.766 -7.895 1.00 52.78 ATOM 5860 CE1 PHE A 374 7.448 -2.766 -7.895 1.00 52.67 ATOM 5866 CD2 PHE A 374 5.326 -2.083 -8.737 1.00 49.05 ATOM 5866 CD2 PHE A 374 5.326 -2.083 -8.737 1.00 49.05 ATOM 5866 CP PHE A 374 5.326 -2.083 -8.737 1.00 49.05 ATOM 5868 CP PHE A 374 8.342 -3.543 -13.556 1.00 57.87 ATOM 5869 O PHE A 374 9.536 -3.729 -13.551 1.00 59.75 ATOM 5867 CG1 VAL A 375 8.440 -3.007 -16.020 1.00 72.14 ATOM 5876 CG1 VAL A 375 8.440 -3.007 -16.020 1.00 72.14 ATOM 5876 CG1 VAL A 375 8.661 -3.444 -18.453 1.00 71.54 ATOM 5880 CG2 VAL A 375 7.514 -5.160 -16.966 1.00 72.18 ATOM 5880 CG2 VAL A 375 7.919 -0.792 -16.840 1.00 72.18 ATOM 5888 C VAL A 375 7.999 -0.792 -16.840 1.00 72.18 ATOM 5898 CA THR A 376 10.08 -1.161 -16.073 1.00 88.14 ATOM 5899 CB THR A 376 10.08 -1.161 -16.073 1.00 88.14 ATOM 5899 CB THR A 376 10.08 -1.161 -16.073 1.00 89.17 ATOM 5899 CG1 THR A 376 11.057 -0.171 -13.804 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.389 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.389 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.389 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 88.70 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 88.70 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.17 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.18 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 89.18 ATOM 5899 CG2 THR A 376 11.550 0.063 -17.399 1.00 | | MOTA | 5848 | | | | | | | | | Ō |
| 10 ATOM 5852 CA PHE A 374 7.578 -3.700 -12.360 1.00 55.44 ATOM 5864 CB PHE A 374 7.709 -2.369 -11.615 1.00 53.01 ATOM 5857 CG PHE A 374 7.709 -2.369 -11.615 1.00 53.01 ATOM 5850 CB1 PHE A 374 7.959 -2.743 -9.179 1.00 47.22 ATOM 5860 CB1 PHE A 374 7.959 -2.743 -9.179 1.00 47.22 ATOM 5860 CB1 PHE A 374 7.959 -2.743 -9.179 1.00 47.22 ATOM 5860 CB2 PHE A 374 6.132 -2.437 -7.669 1.00 52.78 ATOM 5866 CD2 PHE A 374 5.326 -2.083 -8.737 1.00 49.05 ATOM 5860 CD2 PHE A 374 8.342 -3.543 -13.556 1.00 57.87 ATOM 5860 CD PHE A 374 8.342 -3.543 -13.556 1.00 59.75 ATOM 5860 CP PHE A 374 8.342 -3.543 -13.556 1.00 59.75 ATOM 5860 CP PHE A 374 8.342 -3.543 -13.556 1.00 59.75 ATOM 5860 CP PHE A 374 8.342 -3.543 -13.556 1.00 59.75 ATOM 5870 N VAL A 375 7.692 -3.183 -14.762 1.00 68.38 ATOM 5876 CG1 VAL A 375 7.592 -3.656 -17.217 1.00 73.03 ATOM 5876 CG2 VAL A 375 7.752 -3.656 -17.217 1.00 73.03 ATOM 5880 CG2 VAL A 375 7.514 -5.160 -16.966 1.00 72.18 ATOM 5880 CG2 VAL A 375 7.514 -5.160 -16.966 1.00 72.18 ATOM 5880 CG2 VAL A 375 7.599 -0.792 -16.840 1.00 79.60 ATOM 5890 CB THR A 376 10.008 -1.161 -16.073 1.00 79.60 ATOM 5890 CB THR A 376 10.008 -1.161 -16.073 1.00 89.17 ATOM 5890 CB THR A 376 10.008 -1.161 -16.073 1.00 89.17 ATOM 5890 CB THR A 376 11.255 0.740 -14.901 1.00 89.17 ATOM 5890 CB THR A 376 11.255 0.740 -14.901 1.00 89.17 ATOM 5890 CB THR A 376 11.057 -0.171 -13.804 1.00 89.17 ATOM 5890 CB THR A 376 11.564 -1.086 -17.389 1.00 88.23 ATOM 5890 CB THR A 376 11.057 -0.171 -13.804 1.00 89.17 ATOM 5890 CB THR A 376 11.255 0.740 -14.901 1.00 89.17 ATOM 5890 CB THR A 376 11.255 0.740 -14.901 1.00 89.18 ATOM 5890 CB THR A 376 11.255 0.740 -14.901 1.00 89.18 ATOM 5890 CB THR A 376 11.564 -1.086 -17.389 1.00 88.23 ATOM 5890 CB THR A 376 11.564 -1.086 -17.389 1.00 88.23 ATOM 5890 CB THR A 376 11.560 0.063 -17.389 1.00 88.23 ATOM 5890 CB THR A 376 11.560 0.063 -17.389 1.00 89.18 ATOM 5890 CB THR A 376 11.560 0.063 -17.389 1.00 89.80 ATOM 5891 CB A | | MOTA | 5849 | | | | | -6.033 -11.428 | | | | N |
| ATOM S852 CA PHE A 374 7.578 -3.700 -12.360 1.00 53.01 ATOM S854 CB PHE A 374 7.709 -2.369 -11.615 1.00 53.01 ATOM S855 CG PHE A 374 7.163 -2.396 -11.615 1.00 53.01 ATOM S860 CEI PHE A 374 7.163 -2.396 -11.615 1.00 53.01 ATOM S860 CEI PHE A 374 7.448 -2.766 -7.895 1.00 52.78 ATOM S862 CZ PHE A 374 6.132 -2.437 -7.669 1.00 52.76 ATOM S866 CEI PHE A 374 5.326 -2.063 -9.997 1.00 49.05 ATOM S866 CD2 PHE A 374 5.840 -2.063 -9.997 1.00 49.05 ATOM S867 OR PHE A 374 8.342 -3.543 -13.656 1.00 57.87 ATOM S870 N VAL A 375 7.992 -3.183 -14.762 1.00 68.38 ATOM S874 CB VAL A 375 8.440 -3.007 -16.020 1.00 72.14 ATOM S876 CGI VAL A 375 8.440 -3.007 -16.020 1.00 72.14 ATOM S876 CGI VAL A 375 8.440 -3.007 -16.020 1.00 72.14 ATOM S876 CGI VAL A 375 8.440 -3.007 -16.020 1.00 72.14 ATOM S876 CGI VAL A 375 8.757 -1.541 -16.397 1.00 73.03 ATOM S880 CG2 VAL A 375 8.757 -1.541 -16.397 1.00 79.60 ATOM S888 C VAL A 375 7.909 -0.792 -16.840 1.00 79.60 ATOM S888 C VAL A 376 10.008 -1.161 -16.073 1.00 81.14 ATOM S890 CM THR A 376 10.008 -1.161 -16.073 1.00 81.14 ATOM S890 CM THR A 376 11.057 -0.171 -13.804 1.00 80.70 ATOM S890 CM THR A 376 11.057 -0.171 -13.804 1.00 80.70 ATOM S890 CM THR A 376 11.057 -0.171 -13.804 1.00 80.70 ATOM S890 CM THR A 376 11.057 -0.171 -13.804 1.00 80.70 ATOM S890 CM THR A 376 11.050 -0.068 -1.7399 1.00 80.70 ATOM S990 CM LEU A 377 12.144 1.155 -17.922 1.00 80.70 ATOM S990 CM LEU A 377 1.1.500 -0.068 -1.7399 1.00 80.70 ATOM S990 CM LEU A 377 12.500 -1.199 1.00 90.35 ATOM S990 CM | | ATOM | 5850 | N | PHE A 374 | | | -4.797 -11.584 | | | | c |
| ATOM 5854 CB PHE A 374 | 10 | | 5852 | CA | PHE A 374 | | 7.578 | | | | | c |
| ATOM 5857 CG PHE A 374 | 10 | | 5854 | CB | PHE A 374 | | 7.709 | -2.369 -11.615 | | | | |
| ATOM 5858 CDI PHE A 374 | | | | | | | 7.163 | -2.396 -10.227 | | | | C |
| ATOM 5860 CE1 PHE A 374 | • | | | | | | 7.959 | -2.743 - 9.179 | | | | C |
| 15 ATOM 5862 CZ PHE A 374 | | | | | | | 7.448 | -2.766 - 7.895 | | | | С |
| ATOM 5864 CE2 PHE A 374 | 15 | | | | | | 6.132 | -2.437 - 7.669 | | | | С |
| ATOM 5866 CD2 PHE A 374 ATOM 5866 CD2 PHE A 374 ATOM 5869 O PHE A 374 ATOM 5870 N VAL A 375 ATOM 5871 CA VAL A 375 ATOM 5872 CA VAL A 375 ATOM 5876 CG1 VAL A 375 ATOM 5876 CG1 VAL A 375 ATOM 5876 CG2 VAL A 375 ATOM 5880 CG2 VAL A 375 ATOM 5880 CG2 VAL A 375 ATOM 5880 C VAL A 376 ATOM 5880 C VAL A 376 ATOM 5890 C VAL A 376 ATOM 5900 N LEU A 377 ATOM 5900 N LEU A 377 ATOM 5901 C VAL A 376 ATOM 5901 C VAL A 377 ATOM 5902 C VAL A 377 ATOM 5901 C VAL A 377 ATOM 5902 C VAL A 377 ATOM 5903 C VAL A 377 ATOM 5 | 13 | • | | | | | | | | | | С |
| ATOM 5866 C PHE A 374 | | | | | | | | | 1.00 49.61 | | | С |
| ATOM 5869 O PHE A 374 9.556 -3.729 -13.651 1.00 59.75 ATOM 5870 N VAL A 375 7.692 -3.183 -14.762 1.00 68.38 ATOM 5870 CA VAL A 375 7.692 -3.183 -14.762 1.00 72.14 ATOM 5876 CB VAL A 375 8.440 -3.007 -16.020 1.00 72.14 ATOM 5876 CG1 VAL A 375 8.661 -3.444 -18.453 1.00 71.54 ATOM 5880 CG2 VAL A 375 7.514 -5.160 -16.966 1.00 72.18 ATOM 5886 C VAL A 375 7.514 -5.160 -16.966 1.00 72.18 ATOM 5886 N THR A 376 10.008 -1.161 -16.373 1.00 85.14 ATOM 5888 CA THR A 376 10.008 -1.161 -16.073 1.00 85.14 ATOM 5888 CA THR A 376 10.008 -1.161 -16.073 1.00 85.14 ATOM 5890 CB THR A 376 11.255 0.740 -14.901 1.00 89.17 ATOM 5894 CG2 THR A 376 11.057 -0.171 -13.804 1.00 89.17 ATOM 5899 C THR A 376 11.057 -0.171 -13.804 1.00 86.17 ATOM 5899 C THR A 376 11.560 0.063 -17.389 1.00 88.70 ATOM 5900 N LEU A 377 12.114 1.155 -17.922 1.00 87.83 ATOM 5900 CG LEU A 377 12.114 1.155 -17.922 1.00 87.83 ATOM 5904 CB LEU A 377 12.510 1.234 -20.409 1.00 88.50 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.96 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5910 C C G ASP A 378 15.250 -1.159 -21.579 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5910 C ASP A 378 15.250 -1.159 -21.579 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5910 C C G ASP A 378 15.250 -1.159 -21.579 1.00 90.81 ATOM 5910 C C G ASP A 378 17.513 1.894 -22.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5910 C C G ASP A 378 17.513 1.894 -22.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5910 C C G ASP A 378 17.513 1.894 -22.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.75 ATOM 5913 N MET A 379 15.525 -1.159 -1.159 -1.00 90.81 ATOM 5913 N MET A 379 15.525 -1.159 -1.00 90.81 ATOM 5920 C ASP A 378 17.513 1.894 -20.006 1.00 95.71 ATOM 5931 C MET A 379 15.006 -1. | | | | | | | | | 1.00 57.87 | | | С |
| ATOM 5870 N VAL A 375 | | | | | | | | -3 729 -13.651 | | | | 0 |
| ATOM 5872 CA VAL A 375 | | | | | | | | | | | | N |
| ATOM 5874 CB VAL A 375 7.752 -3.656 -17.217 1.00 73.03 ATOM 5876 CG1 VAL A 375 8.601 -3.444 -18.453 1.00 71.54 ATOM 5880 CG2 VAL A 375 7.514 -5.160 -16.966 1.00 72.18 ATOM 5885 O VAL A 375 7.909 -0.792 -16.840 1.00 79.60 ATOM 5886 N THR A 376 10.058 -1.161 -16.073 1.00 85.14 ATOM 5888 CA THR A 376 10.529 0.219 -16.248 1.00 88.23 ATOM 5890 CB THR A 376 11.255 0.740 -14.901 1.00 89.17 ATOM 5892 OGI THR A 376 11.057 -0.171 -13.804 1.00 90.48 ATOM 5899 O THR A 376 11.657 -0.171 -13.804 1.00 88.70 ATOM 5899 O THR A 376 11.560 0.063 -17.389 1.00 86.17 ATOM 5899 O THR A 376 11.664 -1.096 -17.791 1.00 87.38 ATOM 5900 N LEU A 377 12.114 1.155 -17.922 1.00 87.83 ATOM 5900 CB LEU A 377 12.510 1.234 -20.409 1.00 89.85 ATOM 5907 CG LEU A 377 12.510 1.234 -20.409 1.00 89.86 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 1.234 -20.409 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.550 -1.159 -21.579 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.520 -1.159 -21.579 1.00 90.81 ATOM 5913 CD2 LEU A 377 12.520 -1.159 -21.579 1.00 90.81 ATOM 5913 N ASP A 378 17.522 -1.159 -21.579 1.00 90.81 ATOM 5913 N ASP A 378 17.528 1.480 -19.937 1.00 92.45 ATOM 5923 CB ASP A 378 17.513 1.894 -22.480 1.00102.00 ATOM 5928 OD2 ASP A 378 17.513 1.894 -22.480 1.00102.00 ATOM 5933 CB MET A 379 15.163 -1.374 -1.259 1.00 66.38 ATOM 5933 CB MET A 379 15.163 -1.374 -1.259 1.00 68.39 ATOM 5934 CB MET A 379 15.163 -1.374 -1.259 1.00 66.38 ATOM 5940 CB MET A 379 15.285 -1.460 0.455 -16.607 1.00 99.3 ATOM 5940 CB MET A 379 15.28 | 20 | | | | | | 0.440 | | | | | C |
| ATOM 5876 CG1 VAL A 375 | | | | | | | | | | | | С |
| ATOM 5880 CG2 VAL A 375 | • | ATOM | | | | | | | | | | С |
| 25 ATOM 5884 C VAL A 375 | • | MOTA | 5876 | | | | | | | | | Ċ |
| ATOM 5885 O VAL A 375 | | MOTA | 5880 | CG2 | | | 7.514 | | | | | Ċ |
| ATOM 5885 O VAL A 375 ATOM 5886 N THR A 376 ATOM 5888 CA THR A 376 ATOM 5890 CB THR A 376 ATOM 5892 OGI THR A 376 ATOM 5894 CG2 THR A 376 ATOM 5894 CG2 THR A 376 ATOM 5898 C THR A 376 ATOM 5899 O THR A 376 ATOM 5890 N LEU A 377 ATOM 5900 N LEU A 377 ATOM 5900 CB LEU A 377 ATOM 5907 CB LEU A 377 ATOM 5909 CD LEU A 377 ATOM 5918 C LEU A 377 ATOM 5918 O LEU A 377 ATOM 5918 O LEU A 377 ATOM 5919 N ASP A 378 ATOM 5922 CA ASP A 378 ATOM 5922 CA ASP A 378 ATOM 5923 CB ASP A 378 ATOM 5924 CB ASP A 378 ATOM 5925 CB ASP A 378 ATOM 5926 CG ASP A 378 ATOM 5927 ODI ASP A 378 ATOM 5928 OD2 ASP A 378 ATOM 5930 C ASP A 378 ATOM 5931 CB ASP A 378 ATOM 5932 CB ASP A 378 ATOM 5934 CB ASP A 378 ATOM 5935 CB MET A 379 ATOM 5930 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5926 CB ASP A 378 ATOM 5927 ODI ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5931 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5931 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5931 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5931 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5931 CB ASP A 378 ATOM 5930 CB ASP A 378 ATOM 5931 CB ASP A 378 ATOM 5932 CB ASP A 378 ATOM 5933 CB ASP A 378 ATOM 5934 CB ASP A 379 ATOM 5936 CB ASP A 379 ATOM 5946 | 25 | ATOM | 5884 | С | VAL A 375 | | | | | | | ŏ |
| ATOM 5888 CA THR A 376 | | ATOM | 5885 | 0 | | | 7.909 | | | | | N |
| ATOM 5890 CB THR A 376 | | ATOM | 5886 | N | | • | | -1.161 -16.073 | | | | C |
| ATOM 5890 CB THR A 376 | | ATOM | 5888 | CA | THR A 376 | | 10.529 | | | | | |
| ATOM 5892 CG2 THR A 376 11.057 -0.171 -13.804 1.00 90.48 ATOM 5898 C THR A 376 11.560 0.063 -17.389 1.00 88.70 ATOM 5899 O THR A 376 11.560 0.063 -17.389 1.00 88.70 ATOM 5899 O THR A 376 11.864 -1.086 -17.791 1.00 87.38 ATOM 5900 N LEU A 377 12.114 1.155 -17.922 1.00 87.83 ATOM 5902 CA LEU A 377 12.114 1.155 -17.922 1.00 87.83 ATOM 5904 CB LEU A 377 12.510 1.234 -20.409 1.00 90.35 ATOM 5909 CD1 LEU A 377 12.510 1.234 -20.409 1.00 89.96 ATOM 5913 CD2 LEU A 377 12.520 -1.159 -21.579 1.00 89.80 ATOM 5917 C LEU A 377 12.520 -1.159 -21.579 1.00 89.80 ATOM 5918 O LEU A 377 14.475 1.712 -18.873 1.00 89.75 ATOM 5918 O LEU A 377 14.475 1.712 -18.873 1.00 89.75 ATOM 5919 N ASP A 378 15.258 1.480 -19.937 1.00 92.45 ATOM 5921 CA ASP A 378 15.258 1.480 -19.937 1.00 92.45 ATOM 5922 CB ASP A 378 17.018 2.767 -21.238 1.00 98.28 ATOM 5923 CB ASP A 378 17.018 2.767 -21.238 1.00 98.28 ATOM 5926 CG ASP A 378 17.062 2.143 -23.628 1.00101.56 ATOM 5928 OD2 ASP A 378 17.062 2.143 -23.628 1.00101.56 ATOM 5929 C ASP A 378 17.057 3.589 -18.295 1.00 96.63 ATOM 5931 N MET A 379 16.945 1.359 -17.798 1.00 91.54 ATOM 5933 CB MET A 379 16.945 1.359 -17.798 1.00 93.99 ATOM 5940 CB MET A 379 15.410 -0.062 -15.499 1.00 66.38 ATOM 5940 O MET A 379 15.410 -0.062 -15.998 1.00 67.19 ATOM 5940 O MET A 379 15.410 -0.062 -15.998 1.00 69.93 ATOM 5947 O MET A 379 15.420 -0.615 -17.575 1.00 90.93 ATOM 5948 N GLU A 380 21.180 0.455 -16.602 1.00 93.24 ATOM 5950 CB GLU A 380 21.180 0.455 | | | | СВ | THR A 376 | | | | | | Ċ | C |
| ATOM 5894 CG2 THR A 376 | 30 | | | OG1 | THR A 376 | - | 11.057 | | | | | 0 |
| ATOM 5898 C THR A 376 | 50 | - | | | | | 10.674 | 1.992 -14.352 | | • | | C |
| ATOM 5899 O THR A 376 ATOM 5900 N LEU A 377 12.114 1.155 -17.922 1.00 87.83 ATOM 5902 CA LEU A 377 13.111 0.969 -18.996 1.00 88.50 ATOM 5904 CB LEU A 377 12.510 1.234 -20.409 1.00 90.35 ATOM 5907 CG LEU A 377 12.510 1.234 -20.409 1.00 89.96 ATOM 5909 CD1 LEU A 377 12.510 1.234 -20.409 1.00 89.96 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.80 ATOM 5913 CD2 LEU A 377 12.520 -1.159 -21.579 1.00 90.81 ATOM 5918 O LEU A 377 14.475 1.712 -18.873 1.00 89.75 ATOM 5919 N ASP A 378 15.258 1.480 -19.937 1.00 82.52 ATOM 5921 CA ASP A 378 17.018 2.767 -21.238 1.00 92.45 ATOM 5923 CB ASP A 378 17.018 2.767 -21.238 1.00 92.45 ATOM 5926 CG ASP A 378 17.018 2.767 -21.238 1.00 98.28 ATOM 5927 OD1 ASP A 378 17.062 2.143 -23.628 1.00101.56 ATOM 5928 OD2 ASP A 378 17.062 2.143 -23.628 1.00101.56 ATOM 5929 C ASP A 378 16.922 2.405 -18.610 1.00 94.33 ATOM 5930 O ASP A 378 16.922 2.405 -18.610 1.00 96.66 50 ATOM 5931 N MET A 379 16.910 -0.019 -15.863 1.00 87.83 51 ATOM 5938 CG MET A 379 15.410 -0.082 -15.499 1.00 66.38 ATOM 5940 C MET A 379 15.285 -2.746 -15.258 1.00 67.19 ATOM 5940 C MET A 379 15.285 -2.746 -15.258 1.00 67.19 ATOM 5946 C MET A 379 15.285 -2.746 -15.259 1.00 66.38 ATOM 5947 O MET A 379 15.285 -2.746 -15.259 1.00 69.93 ATOM 5948 N GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 | | | | | | | 11.560 | 0.063 -17.389 | | | | С |
| ATOM 5900 N LEU A 377 12.114 1.155 -17.922 1.00 87.83 ATOM 5902 CA LEU A 377 13.111 0.969 -18.996 1.00 88.50 ATOM 5907 CG LEU A 377 12.510 1.234 -20.409 1.00 90.35 ATOM 5909 CD1 LEU A 377 12.034 0.935 -22.783 1.00 89.80 ATOM 5913 CD2 LEU A 377 12.034 0.935 -22.783 1.00 89.80 ATOM 5917 C LEU A 377 12.520 -1.159 -21.579 1.00 90.81 ATOM 5918 O LEU A 377 14.475 1.712 -18.873 1.00 89.75 ATOM 5919 N ASP A 378 15.258 1.480 -19.937 1.00 92.45 ATOM 5921 CA ASP A 378 16.640 1.894 -20.006 1.00 95.71 ATOM 5923 CB ASP A 378 17.018 2.767 -21.238 1.00 98.28 45 ATOM 5926 CG ASP A 378 17.018 2.767 -21.238 1.00 98.28 ATOM 5927 OD1 ASP A 378 17.062 2.143 -23.628 1.00101.56 ATOM 5928 OD2 ASP A 378 16.922 2.405 -18.610 1.00 94.33 ATOM 5930 O ASP A 378 16.922 2.405 -18.610 1.00 94.33 ATOM 5931 N MET A 379 16.945 1.359 -17.798 1.00 91.54 ATOM 5933 CA MET A 379 16.945 1.359 -17.798 1.00 91.54 ATOM 5933 CA MET A 379 16.945 1.359 -17.798 1.00 91.54 ATOM 5935 CB MET A 379 15.265 1.328 -16.436 1.00 87.87 ATOM 5936 CG MET A 379 15.285 -2.746 -15.258 1.00 66.38 ATOM 5937 O MET A 379 15.285 -2.746 -15.258 1.00 67.19 ATOM 5946 C MET A 379 15.285 -2.746 -15.258 1.00 89.93 ATOM 5946 C MET A 379 19.336 2.602 -15.998 1.00 89.93 ATOM 5948 N GLU A 380 21.180 0.455 -16.602 1.00 90.93 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5952 CB GLU A 380 21.180 0.455 -16.602 1.00 93.24 | | | | | | | | -1.086 -17.791 | | | | 0 |
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| ATOM 5933 CA MET A 379 ATOM 5935 CB MET A 379 ATOM 5938 CG MET A 379 ATOM 5941 SD MET A 379 ATOM 5942 CE MET A 379 ATOM 5946 C MET A 379 ATOM 5946 C MET A 379 ATOM 5947 O MET A 379 ATOM 5948 N GLU A 380 ATOM 5950 CA GLU A 380 ATOM 5952 CB GLU A 380 ATOM 5953 CB GLU A 380 ATOM 5954 ATOM 5952 CB GLU A 380 ATOM 5955 CB GLU A 380 ATOM 5956 CB GLU A 380 ATOM 5958 ATOM 5956 CB GLU A 380 ATOM 5958 | 50 | MOTA | 5931 | N | MET A 379 | | | 1.359 -17.798 | 1.00 91.54 | | | |
| ATOM 5935 CB MET A 379 ATOM 5938 CG MET A 379 ATOM 5941 SD MET A 379 ATOM 5942 CE MET A 379 ATOM 5946 C MET A 379 ATOM 5947 O MET A 379 ATOM 5948 N GLU A 380 ATOM 5950 CA GLU A 380 ATOM 5952 CB GLU A 380 AT | | | 5933 | CA | | | | | | | | C |
| ATOM 5938 CG MET A 379 15.410 -0.082 -15.499 1.00 78.36 ATOM 5941 SD MET A 379 15.163 -1.374 -14.259 1.00 66.38 55 ATOM 5942 CE MET A 379 15.285 -2.746 -15.258 1.00 67.19 ATOM 5946 C MET A 379 18.885 1.495 -16.353 1.00 89.93 ATOM 5947 O MET A 379 19.336 2.602 -15.998 1.00 89.20 ATOM 5948 N GLU A 380 19.666 0.432 -16.667 1.00 90.93 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 | | | | CB | MET A 379 | | 16.910 | | | | | C |
| ATOM 5941 SD MET A 379 15.163 -1.374 -14.259 1.00 66.38 55 ATOM 5942 CE MET A 379 15.285 -2.746 -15.258 1.00 67.19 ATOM 5946 C MET A 379 18.885 1.495 -16.353 1.00 89.93 ATOM 5947 O MET A 379 19.336 2.602 -15.998 1.00 89.20 ATOM 5948 N GLU A 380 19.666 0.432 -16.667 1.00 90.93 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5952 CB GLU A 380 21.820 -0.615 -17.575 1.00 92.65 | | | | CG | | | 15.410 | | | | | C |
| 55 ATOM 5942 CE MET A 379 15.285 -2.746 -15.258 1.00 67.19 ATOM 5946 C MET A 379 18.885 1.495 -16.353 1.00 89.93 ATOM 5947 O MET A 379 19.336 2.602 -15.998 1.00 89.20 ATOM 5948 N GLU A 380 19.666 0.432 -16.667 1.00 90.93 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5952 CB GLU A 380 21.820 -0.615 -17.575 1.00 92.65 | | | | | | | | | | | | S |
| ATOM 5946 C MET A 379 18.885 1.495 -16.353 1.00 89.93 ATOM 5947 O MET A 379 19.336 2.602 -15.998 1.00 89.20 ATOM 5948 N GLU A 380 19.666 0.432 -16.667 1.00 90.93 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5952 CB GLU A 380 21.820 -0.615 -17.575 1.00 92.65 | 55 | | | | | | | -2.746 -15.25 | | | | С |
| ATOM 5947 O MET A 379 19.336 2.602 -15.998 1.00 89.20 ATOM 5948 N GLU A 380 19.666 0.432 -16.667 1.00 90.93 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5952 CB GLU A 380 21.820 -0.615 -17.575 1.00 92.65 | رر | | | | | | | 1.495 -16.35 | 3 1.00 89.93 | | | С |
| ATOM 5948 N GLU A 380 19.666 0.432 -16.667 1.00 90.93 ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5952 CB GLU A 380 21.820 -0.615 -17.575 1.00 92.65 | | | | | MET A 379 | | | | | | | · 0 |
| ATOM 5950 CA GLU A 380 21.180 0.455 -16.602 1.00 93.24 60 ATOM 5952 CB GLU A 380 21.820 -0.615 -17.575 1.00 92.65 | | | | | OBE & ILL | | | | | | | N |
| 60 ATOM 5952 CB GLU A 380 21.820 -0.615 -17.575 1.00 92.65 | | | | | CIII V 38U | | | | | | | С |
| 00 Alon 030 22 205 1 221 -17 244 1 00 91 21 | C 0 | | | | GTO V 200 | | | | | | | С |
| ATOM 5955 CG GLU A 500 25.205 1.251 1.151 1.100 51.21 | Oυ | | | | GTO W 200 | | | | | | | С |
| | | MOTA | 5955 | - CG | GLU H 200 | | 43,403 | 1 1 | | | | |

| 5 | ATOM | | | SLU A. | | 23.355 | -1.819 -15 | | 1.00 9 | | | C O |
|-----|------|------|-------|--------|-----|--------|------------|--------|--------|-------|----|--------|
| | MOTA | | | SLU A | | | -3.027 -15 | | 1.00 8 | | ٠. | 0 - |
| | MOTA | 5960 | | SLU A | | 23.811 | -1.058 -14 | | 1.00 9 | | | Č |
| | MOTA | 5961 | | SLU A | | 21.762 | 1.922 -16 | | 1.00 9 | | | Ö |
| • | MOTA | 5962 | | SLU A | | 22.744 | 2.305 -16 | | 1.00 9 | | | N |
| 10 | MOTA | 5963 | | ASP A | | 21.142 | 2.717 -17 | | 1.00 9 | | | C |
| | ATOM | 5965 | | ASP A | | 21.428 | 4.156 -1 | | 1.00 8 | | | C |
| | | 5967 | CB A | ASP A | 381 | 20.206 | 4.883 -18 | | 1.00 | | | C |
| | ATOM | 5970 | | ASP A | | 19.817 | 4.397 -19 | 9.774 | 1.00 | | | |
| | MOTA | 5971 | OD1 A | ASP A | 381 | 20.728 | 4.002 -20 | | 1.001 | | | 0 |
| 15 | MOTA | 5972 | OD2 Z | ASP A | 381 | 18.627 | 4.380 -20 | | | 96.62 | | C |
| | MOTA | 5973 | C Z | ASP A | 381 | 21.691 | 4.860 -1 | | 1.00 | | | |
| | ATOM | 5974 | 0 . 2 | ASP A | 381 | 22.594 | 5.688 -1 | | 1.00 | | | 0 |
| | ATOM | 5975 | N . (| CYS A | 382 | 20.883 | 4.521 -1 | 5.540 | 1.00 | | | N |
| • | ATOM | 5977 | CA (| CYS A | 382 | 20.891 | 5.209 -1 | | 1.00 | | | С |
| 20 | ATOM | 5979 | CB (| CYS A | 382 | 19.874 | 4.543 - 1 | | 1.00 | • | | C |
| ~~ | MOTA | 5982 | SG | CYS A | 382 | 18.314 | 4.339 -1 | | 1.00 | | | S |
| | ATOM | 5983 | | CYS A | | 22.273 | | | 1.00 | | | C |
| | ATOM | 5984 | | CYS A | | 22.585 | 5.663 -1 | | 1.00 | | • | 0 |
| | ATOM | 5985 | | GLY A | | 23.123 | 4.433 -1 | | 1.00 | | | Ņ |
| 25 | ATOM | 5987 | | GLY A | | 24.478 | 4.336 -1 | 4.011 | | 66.26 | | C |
| 23 | ATOM | 5990 | | GLY A | | 25.143 | 5.670 -1 | | | 69.13 | | C |
| | ATOM | 5991 | | GLY A | 383 | 25.005 | 6.281 -1 | | | 70.50 | | 0 |
| | ATOM | 5992 | | TYR A | | 25.854 | 6.144 -1 | | | 73.69 | | N |
| | ATOM | 5994 | | TYR A | | 26.709 | 7.277 -1 | | | 77.96 | | C |
| 30 | ATOM | 5996 | | TYR A | | 26.793 | 8.188 -1 | | | 81.61 | | C |
| 50 | ATOM | 5999 | | TYR A | | 28.007 | 9.089 -1 | | | 85.12 | | C |
| | ATOM | 6000 | | TYR A | | 27.941 | 10.364 -1 | 2.854 | | 88.82 | | C |
| | MOTA | 6002 | | TYR A | | 29.048 | 11.194 -1 | | | 87.19 | | C |
| | MOTA | 6004 | | TYR A | | 30.239 | 10.752 -1 | | | 90.20 | | C |
| 35 | ATOM | 6005 | | TYR A | | 31.364 | 11.553 -1 | | | 89.10 | | 0 |
| 55 | ATOM | 6007 | | TYR A | | 30.320 | 9.490 -1 | | | 90.57 | | C · |
| | ATOM | 6009 | | TYR A | | 29.208 | 8.670 -1 | | | 84.83 | | C |
| | ATOM | 6011 | С | TYR A | | 28.056 | 6.649 -1 | | | 77.71 | ٠ | . C |
| | ATOM | 6012 | 0 | TYR A | 384 | 28.429 | 5.664 -1 | 13.131 | | 75.56 | | 0 |
| 40 | MOTA | 6013 | N | ASN A | | 28.780 | 7.220 - | | | 80.96 | | N |
| •• | MOTA | | CA | ASN A | | 30.051 | 6.662 - | | | 82.76 | | C |
| | ATOM | 6017 | СВ | ASN A | | 29.941 | 6.194 -1 | | | 84.72 | | C |
| | ATOM | 6020 | CG | ASN A | 385 | 29.453 | 4.740 - | | | 87.65 | | С |
| | ATOM | 6021 | OD1 | ASN A | | 30.172 | 3.790 - | | | 85.93 | | 0 |
| 45 | ATOM | 6022 | | ASN A | | 28.236 | 4.570 - | | | 88.07 | • | N |
| | ATOM | 6025 | С | ASN A | | 31.164 | 7.705 - | | | 83.09 | | C |
| | ATOM | 6026 | 0 | ASN A | | 30.936 | 8.930 - | | | 81.57 | | 0 |
| | ATOM | 6027 | OXT | ASN A | | 32.333 | 7.337 - | 14.908 | | 82.17 | | 0 |
| | ATOM | | N | SER E | -2 | 27.206 | 72.118 | 43.679 | | 55.48 | | N |
| 50 | MOTA | 6030 | CA | SER E | | 27.761 | | 43.412 | | 51.63 | | C. |
| 50 | ATOM | 6032 | СВ | SER E | | 29.098 | 73.250 | 42.712 | 1.00 | 52.68 | | С |
| | ATOM | 6035 | OG | SER E | | 29.217 | 71.863 | 42.380 | | 49.83 | | 0 |
| . 1 | ATOM | 6037 | c | SER E | | 26.787 | 74.421 | 42.623 | | 54,62 | | C |
| | ATOM | 6038 | 0 | SER E | | 26.955 | | 42.639 | | 56.38 | | 0 |
| 55 | ATOM | 6041 | N | PHE E | | 25.784 | 73.900 | 41.916 | | 57.53 | | N |
| رر | ATOM | 6043 | CA | PHE E | | 24.690 | | 41.393 | 1.00 | 57.72 | | С |
| | ATOM | 6045 | CB | PHE I | | 24.532 | | 39.920 | | 56.01 | | C |
| | ATOM | 6048 | CG | PHE I | | 25.795 | | 39.141 | | 51.92 | | С |
| | ATOM | 6049 | | PHE I | | 26.898 | | 39.389 | | 50.49 | | C. |
| 60 | ATOM | 6051 | | PHE I | | 28.085 | | 38.686 | 1.00 | 55.85 | | С |
| 00 | ATOM | 6053 | | PHE | | 28.179 | | 37.725 | 1.00 | 54.01 | | С |
| | HIOH | | | | | | | | | | | |

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27.077
                                                75.840
                                                         37.470
                                                                  1.00 55.50
                                                                                         C
                   CE2 PHE B
                               -1
     MOTA
             6055
                                                                  1.00 50.57
                                                                                         C
                   CD2 PHE B
                               -1
                                        25.888
                                                75.657
                                                         38.182
     ATOM.
             6057
                                                                  1.00 61.06
                                                         42.061
                                                 74.634
     MOTA
             6059
                   C
                       PHE B
                               -1
                                        23.294
                                                                  1.00 68.12
                                                         41.364
                                        22.332
                                                74.340
                       PHE B
                               -1
     MOTA
             6060
                   0
                                                                  1.00 62.33
                                0
                                        23.176
                                                74.848
                                                         43.380
                       VAL B
     MOTA
             6061
                   N
                                                                                         C
                                                                  1.00 58.16
                                0
                                        21.896
                                                74.751
                                                         44.116
10
             6063 CA
                       VAL B
     MOTA
                                                                                         С
                                        21.965
                                                         45.528
                                                                  1.00 61.92
                       VAL B
                                0
                                                 75.382
                   CB
     MOTA
             6065
                                                                                         С
                                                                  1.00 61.26
                       VAL B
                                0
                                        22.579
                                                 74.434
                                                         46.564
             6067
                   CG1
     MOTA
                                                                  1.00 64.85
                                                                                         C
             6071
                   CG2 VAL B
                                0
                                        22.697
                                                 76.717
                                                         45.480
     MOTA
                                                                                         C
                                                                  1.00 59.05
                                        20.728
                                                 75.507
                                                         43.571
     MOTA
             6075
                   C
                       VAL B
                                0
                                                 75.100
                                                                  1.00 64.61
                                        19.588
                                                         43.748
15
             6076
                       VAL B
                                0
     MOTA
                   0
                                        20.973
                                                 76.632
                                                         42.925
                                                                  1.00 61.72
     MOTA
             6077
                   N
                       GLU B
                                1
                                                                  1.00 57.96
                                                                                         С
                                        19.857
                                                 77.434
                                                         42.461
                       GLU B
                                1
     ATOM
             6079
                   CA
                                                 78.617
                                                         41.603
                                                                  1.00 57.40
                                                                                         C
                                        20.322
                       GLU B
     MOTA
             6081
                   CB
                                1
                                                                  1.00 58.84
                                                                                         C
                       GLU B
                                        21.725
                                                 79.136
                                                         41.914
     ATOM
             6084
                                1
                   CG
                                                                  1.00 60.23
                                                                                         C
                                        22.786
                                                 78.540
                                                         41.002
20
     ATOM
             6087.
                   CD
                       GLU B
                                1
                                                                  1.00 67.79
                                                                                         Ø
                                                         40.015
                                        22.369
                                                 77.908
     ATOM
             6088
                   OE1 GLU B
                                1
                                                                  1.00 55.89
                                        24.023
                                                 78.696
                                                         41.244
             6089
                   OE2 GLU B
                                1
     ATOM
                                                 76.490
                                                                  1.00 57.15
                                        19.026
                                                         41.626
                                1
             6090
                   С
                        GLU B
     MOTA
                                                                  1.00 51.98
                                        17.785
                                                 76.566
                                                         41.632
                        GLU B
                                1
     ATOM
             6091
                   0
                                        19.747
                                                 75.587
                                2 .
                                                          40.937
                                                                  1.00 51.73
                                                                                         N
25
                        MET B
     ATOM
             6092
                   N
                                                                  1.00 53.66
                                                                                         С
                       MET B
                                2
                                        19.194
                                                 74.706
                                                         39.908
             6094
                   CA
     ATOM
                                                                  1.00 53.83
                                                                                         С
                                        20.186
                                                 74.649
                                                         38.749
             6096
                   CB
                       MET B
                                2
     ATOM
                                                                                         С
                                                                  1.00 54.04
                                        20.424
                                                 76.043
                                                         38.232
             6099
                   CG
                       MET B
                                2
     ATOM
                                                 76.126
                                                         36.827
                                                                  1.00 61.26
                                        21:390
             6102
                   SD
                        MET B
                                2
     ATOM
                                                                  1.00 61.16
                                                                                         C
                                        22.774
                                                 75.563
                                                         37.449
30
                                2
     MOTA
             6103
                   CE
                       MET B
                                                                                         C
                       MET B
                                                 73.312
                                                          40.298
                                                                  1.00 53.70
                                2
                                        18.775
     MOTA
             6107
                   С
                                                                                         0
                                                                  1.00 60.40
                        MET B
                                2
                                        17.937
                                                 72.707
                                                          39.652
             6108
     MOTA
                   0
                                                                                         N
                                                          41.355
                                                                  1.00 55.79
                                3
                                        19.344
                                                 72.792
             6109
                   N
                        VAL B
     MOTA
                                                                  1.00 54.02
                                                                                         С
                                                          41.806
                        VAL B
                                 3
                                        18.997
                                                 71.464
     MOTA
             6111
                   CA
                                                                                         С
                                                          43.026
                                                                  1.00 55.97
                                        19.858
                                                 71.128
                        VAL B
35
     MOTA
             6113
                   CB
                                3
                                                                                         С
                                        19.458
                                                 69.812
                                                          43.622
                                                                  1.00 56.80
                   CG1 VAL B
                                 3
     ATOM
             6115
                                                                                         С
                                                          42.649
                                                                  1.00 57.96
             6119
                   CG2
                       VAL B
                                 3
                                        21.330
                                                 71.152
     MOTA
                                                                                         C
                                        17.517
                                                                  1.00 52.70
                        VAL B
                                 3
                                                 71.392
                                                          42.216
     ATOM
             6123
                   С
                                                                                         0
                                                          42.812
                                                                  1.00 54.10
             6124
                   o
                        VAL B
                                 3
                                        16.984
                                                 72.320
     ATOM
                                                          41.897
                                                                                         N
                                        16.860
                                                 70.285
                                                                  1.00 54.43
40
                        ASP B
     MOTA
             6125
                   N
                                 4
                                                 70.048
                                                          42.309
                                                                  1.00 58.27
             6127
                    CA
                        ASP B
                                 4
                                        15.474
     MOTA
                                        15.255
                                                                  1.00 62.53
                                                 70.401
                                                          43.793
                        ASP B
     ATOM
             6129
                   CB
                                 4
                                                                                         С
                        ASP B
                                        15.485
                                                 69.206
                                                          44.726
                                                                  1.00 71.31
                   CG
                                 4
     MOTA
             6132
                                                                                         0
                                        15.328
                                                 69.381
                                                          45.965
                                                                  1.00 76.06
                   OD1 ASP B
                                 4
     MOTA
             6133
                                                                                         0
                                                                  1.00 75.48
                                                          44.317
45
             6134
                   OD2
                       ASP B
                                        15.822
                                                 68.060
     MOTA
                                                          41.443
                                                                  1.00 53.53
                                        14.543
                                                 70.851
                        ASP B
     ATOM
             6135
                    С
                                                 71.276
                                                          41.875
                                                                  1.00 51.34
                                        13.461
             6136
                   0
                        ASP B
                                 4
     ATOM
                                                          40.209 1.00 50.18
                                                                                          N
                                        14.978
                                                 71.054
     ATOM
             6137
                   N
                        ASN B
                                 5
                                                          39.290
                                                                  1.00 44.49
                                                                                          С
                                        14.233
                                                 71.893
                        ASN B
                                 5
     MOTA
             6139
                    CA
                                                                                          С
                                 5
                                        15.122
                                                 72.909
                                                          38.651
                                                                  1.00 42.71
50
                        ASN B
                    CB
     ATOM
             6141
                                                                                          C.
                    CG
                        ASN B
                                 5
                                        16.020
                                                 72.302
                                                          37.633
                                                                  1.00 48.45
             6144
     ATOM
                                                                   1.00 41.96
                                                                                          0
                    OD1 ASN B
                                 5
                                        15.983
                                                 71.073
                                                          37.445
      MOTA
             6145
                                                                                          N
                                                          36.946
                                                                   1.00 38.24
             6146
                        ASN B
                                 5
                                         16.850
                                                 73.156
      ATOM
                    ND2
                                                 71.157
                                                          38.209
                                                                   1.00 42.49
                                                                                          C
                        ASN B
                                 5
                                         13.525
             6149
                    С
      MOTA
                                                          37.403
                                                 71.804
                                                                  1.00 52.24
55
                    0
                        ASN B
                                 5
                                         12.928
      MOTA
              6150
                                                  69.826
                                                          38.171
                                                                   1.00 42.05
                                         13.559
      MOTA
              6151
                    N
                        LEU B
                                 6
                                                  69.114
                                                          37.261
                                                                   1.00 39.02
                                         12.673
                        LEU B
                                 6
      ATOM
              6153
                    CA
                                                                                          C.
                        LEU B
                                 6
                                         13.329
                                                  67.894
                                                          36.675
                                                                   1.00 35.91
                    CB
      ATOM
              6155
                                                                                          С
                                         14.619
                                                  68.130
                                                          35.905
                                                                   1.00 35.63
              6158
                    CG
                        LEU B
                                 6
      MOTA
                                                                                          С
                                                          35.207
                    CD1 LEU B
                                         15.044
                                                  66.856
                                                                   1.00 35.19
60
              6160
                                 6
      MOTA
                                                  69.193
                                                          34.893
                                                                  1.00 29.54
                    CD2 LEU B
                                         14.462
              6164
      MOTA
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| | | | | | | | | | | 53 | | | ~ |
|-------------|------|------|-----|-------|-------|----|--------|--------|--------|------------|---|----|-----|
| 5 | MOTA | 6168 | С | LEU | В (| 6 | 11.446 | 68.653 | 37.996 | 1.00 42.53 | | | С |
| | MOTA | 6169 | 0 | LEU ! | В | 6 | 11.394 | 68.726 | 39.205 | 1.00 53.16 | | | 0 |
| | MOTA | 6170 | N | ARG I | в : | 7 | 10.436 | 68.228 | 37.245 | 1.00 42.75 | | | N |
| | MOTA | 6172 | CA | ARG I | в - | 7 | 9.325 | 67.471 | 37.771 | 1.00 38.99 | | | С |
| | ATOM | 6174 | СВ | ARG I | в | 7 | 8.103 | 68.326 | 37.963 | 1.00 41.20 | | | C |
| 10 | ATOM | 6177 | CG | ARG 1 | | 7 | 8.306 | 69.383 | 39.081 | 1.00 48.07 | | | С |
| 10 | ATOM | 6180 | CD | ARG I | | 7 | 7.066 | 70.215 | 39.470 | 1.00 48.13 | | | C |
| | | 6183 | NE | ARG ! | | 7 | 6.508 | 70.882 | 38.289 | 1.00 63.74 | | | N |
| | MOTA | | | | | 7 | 5.417 | 71.659 | 38.262 | 1.00 67.03 | | | C |
| | MOTA | 6185 | CZ | ARG ! | | | | | 39.367 | 1.00 73.42 | | | N |
| | MOTA | 6186 | | ARG I | | 7 | 4.720 | 71.907 | | 1.00 66.22 | | | N |
| 15 | MOTA | 6189 | | ARG : | | 7 | 5.021 | 72.192 | 37.118 | | | | C |
| | MOTA | 6192 | С | ARG : | | 7 | 9.095 | 66.395 | 36.744 | 1.00 41.31 | | | |
| | MOTA | 6193 | 0 | ARG : | | 7 | 9.743 | 66.393 | 35.697 | 1.00 42.80 | | | 0 |
| | MOTA | 6194 | N | GLY : | | В | 8.213 | 65.451 | 37.037 | 1.00 44.24 | | | N |
| | MOTA | 6196 | CA | GLY : | В | В | 7.775 | 64.510 | 36.017 | 1.00 44.58 | | | С |
| 20 | MOTA | 6199 | Ċ | GLY : | в і | В | 8.126 | 63.080 | 36.314 | 1.00 52.57 | | | С |
| • | MOTA | 6200 | Ó | GLY | B . 1 | В | 8.464 | 62.734 | 37.457 | 1.00 54.12 | | | 0 |
| | ATOM | 6201 | N | LYS | В | 9 | 8.059 | 62.251 | 35.270 | 1.00 55.79 | | | N |
| | ATOM | 6203 | CA | LYS | В | 9 | 8.331 | 60.829 | 35.404 | 1.00 58.69 | | | C |
| | ATOM | 6205 | СВ | LYS | | 9 | 7.136 | 60.163 | 36.102 | 1.00 63.35 | | | С |
| 25 | ATOM | 6208 | CG | LYS | | 9 | 5.746 | 60.383 | 35.457 | 1.00 64.18 | | | С |
| 23 | ATOM | 6211 | ĊD | LYS | | 9 | 4.812 | 59.234 | 35.916 | 1.00 65.46 | | | С |
| | ATOM | 6214 | CE | LYS | | 9 | 3.321 | 59.481 | | 1.00 64.84 | | | С |
| | ATOM | 6217 | NZ | LYS | | 9 | 2.630 | 60.116 | 36.794 | 1.00 61.17 | | | N |
| | | 6221 | C | LYS | | | 8.661 | 60.089 | 34.086 | 1.00 59.28 | | | C |
| 2Ò | ATOM | | | LYS | | 9. | 8.631 | 60.659 | 32.990 | 1.00 57.59 | | | ō |
| 30 | MOTA | 6222 | 0 | | | | | | 34.211 | 1.00 57.33 | | | N |
| | ATOM | 6223 | N | SER | | | 8.974 | 58.805 | | 1.00 50.75 | | | C |
| | MOTA | 6225 | CA | SER | | | 9.357 | 57.968 | 33.073 | · · | | | c |
| | ATOM | 6227 | CB | SER | | | 9.764 | 56.630 | 33.631 | 1.00 62.78 | | | o o |
| | ATOM | 6230 | OG | SER | | | 8.858 | 56.310 | | 1.00 64.36 | | | |
| 35 | ATOM | 6232 | C | SER | | | 8.256 | 57.723 | 32.029 | 1.00 62.89 | | | C |
| | MOTA | 6233 | О | SER | | | 8.509 | 57.692 | 30.820 | 1.00 63.54 | | | 0 |
| | MOTA | 6234 | Ŋ | GLY | | 1 | 7.034 | 57.522 | 32.497 | 1.00 60.46 | | | N |
| | MOTA | 6236 | CA | GLY | B 1 | 1 | 5.913 | 57.328 | 31.607 | 1.00 57.59 | | | С |
| | MOTA | 6239 | С | GLY | B 1. | 1 | 5.615 | 58.594 | 30.850 | 1.00 56.83 | | | С |
| 40 | ATOM | 6240 | 0 | GLY | B 1 | 1 | 5.172 | 58.582 | 29.710 | 1.00 59.77 | | | 0 |
| | ATOM | 6241 | N | GLN | B 1 | 2 | 5.855 | 59.731 | 31.456 | 1.00 57.32 | | | N |
| | ATOM | 6243 | CA | GLN | в 1 | 2 | 5.495 | 60.920 | 30.714 | 1.00 58.21 | | | С |
| | ATOM | 6245 | CB | GLN | B 1 | 2 | 4.324 | 61.552 | 31.404 | 1.00 60.77 | | | С |
| | ATOM | 6248 | CG | GLN | в 1 | 2 | 3.241 | 60.485 | 31.587 | 1.00 61.87 | | | С |
| 45 | ATOM | 6251 | CD | GLN | | 2 | 1.931 | 61.070 | 31.972 | 1.00 63.35 | | | C |
| | ATOM | 6252 | | GLN | | 2 | 1.866 | 61.968 | 32.838 | 1.00 64.47 | | | 0 |
| • | ATOM | 6253 | | .GLN | | 2 | 0.862 | 60.578 | 31.346 | 1.00 65.23 | | | N |
| | ATOM | 6256 | | GLN | | 2 | 6.566 | | 30.368 | 1.00 57.52 | | | С |
| | ATOM | 6257 | o. | GLN | | 2 | 6.322 | 62.740 | 29.514 | 1.00 55.14 | | | 0 |
| .50 | | | | | | | 7.747 | 61.848 | 30.973 | 1.00 55.44 | | | N |
| . 50 | MOTA | 6258 | N | GLY | | | 8.778 | 62.837 | 30.689 | 1.00 52.72 | | | C |
| • | ATOM | 6260 | CA | GLY | | 3 | | | | | | | c |
| | ATOM | 6263 | C | GLY | | 3 | 9.039 | 63.777 | | 1.00 51.10 | | | 0 |
| • | ATOM | 6264 | 0 | GLY | | | 8.229 | 63.885 | | 1.00 47.37 | | | |
| | MOTA | 6265 | N | TYR | | 4 | 10.180 | 64.450 | ** | 1.00 47.23 | • | | И |
| 55 . | ATOM | 6267 | CA | TYR | | 4 | 10.685 | • | 32.818 | 1.00 48.86 | | ٠, | C |
| | ATOM | 6269 | CB | TYR | | 4 | 12.079 | 64.874 | 33.266 | 1.00 47.74 | • | | C |
| | ATOM | 6272 | CG | TYR | | 4 | 12.061 | 63.570 | 34.037 | 1.00 45.03 | | | C |
| | ATOM | 6273 | CD1 | TYR | B 1 | 4 | 12.346 | 62.368 | 33.443 | 1.00 45.11 | | | С |
| | MOTA | 6275 | | TYR | | .4 | 12.314 | 61.184 | 34.204 | 1.00 44.50 | | | C |
| 60 | MOTA | 6277 | CZ | TYR | | 4 | 11.978 | 61.258 | 35.556 | 1.00 45.22 | | ٠ | С |
| | ATOM | 6278 | OH | TYR | | 4 | 11.908 | 60.155 | 36.388 | 1.00 45.51 | | | 0 |
| | | | | | _ | | | | | | | | |

| | | | | | | | | | | | | | ~ |
|----|-------|-------|-----|------|----|------|----|--------|--------|--------|------------|---|-----|
| 5 | ATOM | 6280 | CE2 | TYR | В | 14 | | 11.702 | 62.446 | 36.117 | 1.00 37.21 | | С |
| | MOTA | 6282 | CD2 | TYR | В | 14 | | 11.741 | 63.566 | 35.378 | 1.00 43.77 | - | C. |
| | MOTA | 6284 | С | TYR | В | 14 | | 10.776 | 66.739 | 32.217 | 1.00 49.55 | | С |
| | ATOM | 6285 | 0 . | TYR | В | 14 | | 11.293 | 66.888 | 31.111 | 1.00 52.45 | | 0 |
| | ATOM | 6286 | N | TYR | В | 15 | | 10.286 | 67.759 | 32.924 | 1.00 45.83 | | . N |
| 10 | ATOM | 6288 | | TYR | | 15 | | 10.233 | 69.079 | 32.339 | 1.00 39.66 | | С |
| 10 | ATOM | 6290 | | TYR | | 15 | | 8.817 | 69.345 | 31.844 | 1.00 39.42 | | С |
| • | | 6293 | | TYR | | 15 | | 7.835 | 69.394 | 32.978 | 1.00 40.57 | | C |
| | ATOM | | | TYR | | 15 | | 7.743 | 70.510 | 33.798 | 1.00 43.59 | | С |
| | ATOM | 6294 | | | | 15 | | 6.869 | 70.561 | 34.824 | 1.00 34.88 | | С |
| | MOTA | 6296 | | TYR | | | | | 69.496 | 35.062 | 1.00 37.24 | | С |
| 15 | MOTA | 6298 | CZ | TYR | | 15 | | 6.065 | 69.511 | 36.110 | 1.00 47.03 | | ŏ |
| | ATOM | 6299 | | TYR | | 15 | | 5.168 | | 34.273 | 1.00 41.16 | | č |
| | ATOM | 6301 | | TYR | | 15 | | 6.130 | 68.390 | | | | Ċ. |
| | ATOM | 6303 | | | | 15 | | 7.008 | 68.340 | 33.240 | 1.00 42.00 | | |
| | ATOM | 6305 | С | TYR | В | 15 | | 10.686 | 70.194 | 33.276 | 1.00 40.31 | | С |
| 20 | MOTA | 6306 | 0 | TYR | В | 15 | | 10.679 | 70.062 | 34.478 | 1.00 37.96 | | 0 |
| | MOTA | 6307 | N | VAL | В | 16 | | 11.069 | 71.312 | 32.676 | 1.00 43.44 | | N |
| • | MOTA | 6309 | CA | VAL | В | 16 | | 11.673 | 72.427 | 33.369 | 1.00 42.50 | | C |
| | MOTA | 6311 | CB | VAL | В | 16 | | 13.141 | 72.669 | 32.925 | 1.00 40.97 | | С |
| | ATOM | 6313 | | VAĻ | В | 16 | | 13.240 | 73.090 | 31.465 | 1.00 36.56 | | С |
| 25 | ATOM | 6317 | | VAL | | 16 | | 13.724 | 73.752 | 33.699 | 1.00 45.84 | | С |
| 23 | MOTA | 6321 | C | VAL | | .16 | | 10.836 | 73.605 | 32.964 | 1.00 46.17 | | С |
| | ATOM | 6322 | o · | VAL | | 16 | | 10.405 | 73.700 | 31.818 | 1.00 44.78 | | 0 |
| | | 6323 | N | GLU | | 17 | | 10.609 | 74:497 | 33.910 | 1.00 47.27 | | N |
| | ATOM | | | GLU | | 17 | | 9.788 | 75.649 | 33.701 | 1.00 48.45 | | С |
| 20 | ATOM | 6325 | CA | | | 17 | | 9.314 | 76.118 | 35.056 | 1.00 50.22 | | С |
| 30 | ATOM | 6327 | ·CB | GLU | | | | 8.748 | | 35.050 | 1.00 49.63 | | C |
| | ATOM | 6330 | CG | GLU | | 17 | | | | 36.443 | 1.00 52.98 | | Ċ |
| | MOTA | 6333 | CD | GLU | | 17 | | 8.451 | 78.008 | 37.020 | 1.00 56.17 | | ō |
| | ATOM | 6334 | | GLU | | 17 | | 7.420 | 77.598 | | 1.00 62.26 | | ő |
| | MOTA | 6335 | | GLU | | . 17 | | 9.251 | 78.812 | 36.957 | 1.00 49.62 | | c |
| 35 | MOTA | 6336 | С | GLU | | 17 | | 10.587 | 76.771 | 33.070 | · · | | Ö |
| | MOTA | .6337 | 0 | GLU | | 17 | | 11.605 | 77.156 | 33.603 | 1.00 58.28 | • | |
| | MOTA | 6338 | N | MET | В | 18 | | 10.130 | 77.308 | 31.949 | 1.00 52.00 | | N |
| | MOTA | 6340 | CA | MET | В | 18 | | 10.821 | 78.430 | 31.301 | 1.00 52.60 | | C |
| | ATOM | 6342 | CB | MET | В | 18 | | 11.435 | 77.960 | 29.976 | 1.00 52.70 | | C |
| 40 | ATOM | 6345 | CG | MET | В | 18 | | 12.598 | 77.016 | 30.128 | 1.00 55.57 | | C |
| | ATOM | 6348 | SD | MET | B | 18 | | 13.010 | 76.172 | 28.583 | 1.00 59.46 | | S |
| | ATOM | 6349 | CE | МЕТ | В | 18 | | 14.275 | 77.236 | 27.930 | 1.00 52.14 | | С |
| | ATOM | 6353 | С | MET | | 18 | | 9.874 | 79.625 | 31.035 | 1.00 50.66 | | С |
| | ATOM | 6354 | o | MET | | 18 | | 8.647 | 79.496 | 31.067 | 1.00 49.38 | | О |
| 45 | ATOM | 6355 | N | THR | | 19 | | 10.452 | 80.786 | 30.780 | 1.00 49.10 | | N |
| | ATOM | 6357 | CA | THR | | 19 | | 9.650 | 81.918 | 30.382 | 1,00 51.16 | | С |
| | MOTA | 6359 | СВ | THR | ** | 19 | | 9.716 | 83.092 | 31.355 | 1.00 50.92 | | С |
| | | 6361 | OG1 | | | 19 | | 10.956 | 83.832 | 31.217 | 1.00 46.48 | | 0 |
| | ATOM | | | | | | | 9.658 | | | 1.00 52.58 | | C |
| 60 | MOTA | 6363 | | THR | | 19 | | 10.084 | | 29.041 | 1.00 55.56 | | C |
| 50 | MOTA | 6367 | С | THR | | 19 | | | | | | | ō |
| | MOTA | 6368 | 0 | THR | | 19 | | 11.269 | | 28.214 | | | N |
| | MOTA | 6369 | N | VAL | | | ١. | 9.090 | 4.5 | | 1.00 57.24 | | |
| | ATOM | 6371 | CA | VAL | | 20 | | 9.307 | | 26.880 | | | C |
| | ATOM. | 6373 | | VAL | | 20 | | 8.940 | | 25.827 | | | Ċ |
| 55 | ATOM | 6375 | CG1 | VAL | В | 20 | | 9.851 | 80.829 | 25.982 | | | |
| | ATOM | 6379 | CG2 | VAL | В | 20 | | 7.504 | | 25.953 | | | С |
| | ATOM | 6383 | С | VAL | | 20 | | 8.377 | 84.325 | 26.771 | | | С |
| | ATOM | 6384 | 0. | VAL | | 20 | | 7.234 | 84.209 | 27.224 | 1.00 55.85 | | 0 |
| | ATOM | 6385 | N | GLY | | 21 | | 8.875 | | 26.223 | | | N |
| 60 | ATOM | 6387 | CA | GLY | | 21 | | 8.066 | | | | | С |
| 50 | MOTA | 6390 | C | GLY | | 21 | | 8.292 | | | | | С |
| | ATOM | 0550 | ~ | 0.01 | ם | | | 9.252 | | | | | |

| | | | ٠ | | | | | | | | • | | | |
|----|--------|------|------|------|-----|----|--------|--------|--------|--------------------|------|-----|---|-----|
| 5 | ATOM | 6391 | o | GLY | В | 21 | 8.913 | 87.910 | 27.737 | 1.00 4 | 5.49 | | | 0 |
| | ATOM | 6392 | N | SER | В | 22 | 7.772 | 89.020 | 26.147 | 1.00 5 | | | | N |
| | ATOM | 6394 | CA | SER | | 22 | 7.729 | 90.308 | 26.811 | 1.00 4 | | | | C |
| | ATOM | 6396 | CB | SER | | 22 | 8.740 | 91.218 | 26.200 | 1.00 4 | | | | Č |
| | ATOM | 6399 | OG | SER | | 22 | 10.028 | 90.606 | 26.262 | 1.00 5 | | | | Ö |
| 10 | MOTA | 6401 | C | SER | | 22 | 6.328 | 90.918 | 26.679 | 1.00 5 | | | | C |
| 10 | ATOM | 6402 | ō | SER | | 22 | 5.916 | 91.373 | 25.610 | 1.00 3 | | | | |
| | ATOM | 6403 | N | PRO | | 23 | | | | | | | | 0 |
| | ATOM | 6404 | . CA | PRO | | 23 | 5.587 | 90.895 | 27.784 | 1.00 5 | | | | N |
| | ATOM | | | | | | 6.088 | 90.276 | 29.019 | 1.00 5 | | | | C |
| 15 | | 6406 | CB | PRO | | 23 | 4.902 | 90.437 | 29.964 | 1.00 5 | | | | C |
| ίЭ | MOTA | 6409 | CG | PRO | | 23 | 3.759 | 90.424 | 29.043 | 1.00 5 | | | | C |
| • | ATOM | 6412 | CD | PRO | | 23 | 4.226 | 91.436 | 27.979 | 1.00 4 | | | | С |
| | ATOM | 6415 | С | PRO | | 23 | 6.368 | 88.800 | 28.881 | 1.00 4 | | | | С |
| | ATOM | 6416 | 0 | PRO | | 23 | 5.860 | 88.229 | 27.944 | 1.00 4 | | | | 0 |
| 00 | ATOM | 6417 | N | PRO | | 24 | 7.169 | 88.249 | 29.794 | 1.00 5 | | | | N |
| 20 | MOTA | 6418 | CA | PRO | | 24 | 7.415 | 86.787 | 30.020 | 1.00 5 | | | | С |
| | ATOM | 6420 | CB | PRO | | 24 | 8.155 | 86.804 | 31.345 | 1.00 5 | | | | С |
| | ATOM - | 6423 | CG | PRO | | 24 | 8.902 | 88.094 | 31.318 | 1.00 5 | 0.72 | | | С |
| | MOTA | 6426 | CD | PRO | | 24 | 7.995 | 89.088 | 30.680 | 1.00 5 | 3.02 | | | С |
| | ATOM | 6429 | С | PRO | | 24 | 6.260 | 85.781 | 30.261 | 1.00 5 | 5.63 | | | С |
| 25 | MOTA | 6430 | 0 | PRO | | 24 | 5.567 | 85.900 | 31.270 | 1.00 5 | 4.27 | | | 0 . |
| | ATOM | 6431 | N | GLN | B | 25 | 6.097 | 84.775 | 29.392 | 1.00 5 | 7.58 | | | N |
| | MOTA | 6433 | CA | GLN | В | 25 | 5.025 | 83.775 | 29.524 | 1.00 5 | 6.58 | | | . C |
| | ATOM | 6435 | CB | GLN | В | 25 | 4.404 | 83.453 | 28.153 | 1.00 5 | 8.02 | | | C |
| | ATOM | 6438 | .CG | GLN | В | 25 | 3.196 | 84.297 | 27.785 | 1.00 6 | 1.35 | | | С |
| 30 | ATOM | 6441 | CD | GLN | В | 25 | 2.729 | 84.086 | 26.353 | 1.00 6 | 3.09 | | | С |
| • | ATOM | 6442 | OE1 | GLN | В | 25 | 2.293 | 82.981 | 25.990 | 1.00 6 | 9.50 | | | 0 |
| | MOTA | 6443 | NE2 | GLN. | В | 25 | 2.802 | 85.135 | 25.543 | 1.00 5 | 4.51 | | | N |
| | ATOM | 6446 | . C | GLN | В | 25 | 5.604 | 82.496 | 30.116 | 1.00 5 | 8.86 | • • | | С |
| | MOTA | 6447 | 0 | GLN | B∙ | 25 | 6.574 | 81.987 | 29.559 | 1.00 5 | 7.53 | | • | 0 |
| 35 | ATOM | 6448 | N | THR | В | 26 | 5.036 | 82.000 | 31.228 | 1.00 5 | | | | N |
| | ATOM | 6450 | CA | THR | В . | 26 | 5.497 | 80.785 | 31.866 | 1.00 4 | 9.89 | | | С |
| | ATOM | 6452 | CB. | THR | В | 26 | 5.043 | 80.761 | 33.304 | 1.00 5 | 1.53 | | | С |
| • | MOTA | 6454 | OG1 | THR | В | 26 | 5.882 | 81.592 | 34.127 | 1.00 4 | 8.51 | | | 0 |
| | MOTA | 6456 | CG2 | THR | В | 26 | 5.233 | 79.353 | 33.886 | 1.00 4 | 9.37 | | | С |
| 40 | MOTA | 6460 | С | THR | В | 26 | 4.970 | 79.505 | 31.224 | 1.00 5 | 1.74 | | | , C |
| | MOTA | 6461 | 0 | THR | В | 26 | 3.772 | 79.321 | 31.123 | 1.00 5 | 5.36 | | | . 0 |
| | MOTA | 6462 | N | LEU | B . | 27 | 5.861 | 78.603 | 30.808 | 1.00 5 | 2.47 | | | N |
| | ATOM | 6464 | CA | LEU | В | 27 | 5.440 | 77.291 | 30.296 | 1.00 5 | | | | С |
| | ATOM | 6466 | CB | LEU | В. | 27 | 5.447 | 77.292 | 28.768 | 1.00 5 | | | | С |
| 45 | ATOM | 6469 | CG | LEU | В | 27 | 4.766 | 78.485 | 28.088 | 1.00 5 | 5.67 | | | С |
| | ATOM | 6471 | CD1 | LEU | B. | 27 | 5.163 | 78.522 | 26.640 | 1.00 5 | | | | C |
| | ATOM | 6475 | CD2 | LEU | В | 27 | 3.248 | 78.447 | 28.216 | 1.00 5 | | | | С |
| | ATOM | 6479 | С | LEU | В | 27 | 6.344 | 76.152 | | 1.00 5 | | | | Ċ |
| | ATOM | 6480 | 0 | LEU | | 27 | 7.492 | 76.415 | 31.190 | 1.00 5 | | | | o |
| 50 | MOTA | 6481 | | ASN | | 28 | 5.809 | 74.922 | 30.863 | 1.00 5 | | | | N |
| | MOTA | 6483 | | ASN | | 28 | 6.518 | 73.711 | 31.292 | 1.00 5 | | | | c |
| | ATOM | 6485 | | ASN | | 28 | 5.526 | 72.700 | 31.940 | 1.00 5 | | | | č |
| | ATOM | 6488 | | ASN | | 28 | 5.260 | 72.950 | 33.449 | 1.00 5 | | | | č |
| | ATOM | 6489 | | ASN | | 28 | 4.145 | 72.685 | 33.961 | 1.00 4 | | | | Ö |
| 55 | ATOM | 6490 | | ASN | | 28 | 6.273 | 73.440 | 34.152 | 1.00 5 | | | | N |
| • | ATOM | 6493 | C | ASN | | 28 | 7.119 | 73.440 | 30.037 | 1.00 5 | | | | C. |
| | ATOM | 6494 | ŏ | ASN | | 28 | 6.411 | 72.858 | 29.040 | 1.00 5 | | | | 0 |
| | ATOM | 6495 | N | ILE | | 29 | 8.385 | 72.602 | 30.082 | 1.00 4 | | | | |
| | ATOM | 6497 | CA | ILE | | 29 | 9.090 | 72.101 | | | | | | N |
| 60 | ATOM | 6499 | CB | ILE | | 29 | 10.096 | 73.201 | 28.430 | 1.00 4: 1.00 4: | | | | C |
| • | ATOM | 6501 | | ILE | | 29 | 9.403 | 74.521 | 28.502 | 1.00 4 | | | | C |
| | | | | | | | 2.403 | 17.361 | 20.302 | 1.00 3 | 0.07 | | | C |

| _ | 20014 | CEO4 | CD1 | ILE E | | 29 | 8.620 | 74.882 | 27.272 | 1.00 35.29 | | | С |
|-----|--------------|--------------|------|------------|---|----------|------------------|---------|--------|------------|---|---|-----|
| 5 | MOTA | 6504 | | ILE E | | 29 | 10.627 | 72.989 | 27.001 | 1.00 45.92 | | | C |
| | ATOM | 6508 | | ILE I | | 29 | 9.834 | 70.738 | 29.020 | 1.00 41.21 | | | С |
| | ATOM | 6512 | | ILE I | | 29 | 10.821 | 70.657 | 29.735 | 1.00 40.42 | | | 0 |
| | ATOM · | 6513 | | LEU I | | 30 | 9.363 | 69.67.9 | 28.344 | 1.00 40.94 | | | N |
| 10 | MOTA | 6514 | | | | 30 | 10.056 | 68.371 | 28.308 | 1.00 42.00 | | | С |
| 10 | MOTA | 6516 | | LEU I | | 30 | 9.450 | 67.507 | 27.215 | 1.00 41.64 | | | C |
| | ATOM | 6518 | | LEU I | | | 9.943 | 66.065 | 27.050 | 1.00 41.51 | | | C |
| | MOTA | 6521 | - | LEU I | | 30 | 8.966 | 65.054 | 27.427 | 1.00 38.45 | | | Ċ |
| | MOTA | 6523 | | LEU ! | | 30 | | 65.805 | 25.617 | 1.00 51.30 | | • | c |
| | ATOM | 6527 | | LEU I | | 30 · | 10.258 | 68.607 | 27.974 | 1.00 46.49 | | | Č |
| 15 | ATOM | 6531 | С | LEU I | | 30 | 11.529 11.849 | 69.519 | 27.220 | 1.00 47.11 | | | ō |
| | ATOM | 6532 | 0 | LEU ! | | 30 | 12.414 | 67.781 | 28.527 | 1.00 46.41 | | | N |
| | ATOM | 6533 | N | VAL I | | 31 | | 67.781 | 28.288 | 1.00 47.73 | • | | C |
| | MOTA | 6535 | | VAL I | | 31 | 13.858 | 67.834 | 29.620 | 1.00 48.19 | | | č |
| | MOTA | 6537 | CB | VAL | | 31 | 14.633 | 67.314 | 29.431 | 1.00 52.74 | | | č |
| 20 | · MOTA | 6539 | | VAL | | 31 | 16.047 | 69.187 | 30.226 | 1.00 47.82 | | | Č |
| | ATOM | 6543 | | VAL | | 31 | 14.661 | 66.709 | 27.422 | 1.00 49.66 | | | č |
| | ATOM | 6547 | C | VAL | | 31 | 14.251 | 65.614 | 27.935 | 1.00 49.00 | | | ō |
| | MOTA | 6548 | 0 | VAL | | 31 | 14.369 | 66.937 | 26.122 | 1.00 50.95 | | | N |
| 0.5 | ATOM | 6549 | | ASP | | 32 | 14.488 14.599 | 65.825 | 25.165 | 1.00 50.66 | | | C |
| 25 | ATOM | 6551 | CA | ASP | | 32 | 13.547 | | 24.085 | 1.00 46.26 | | | Ċ |
| | MOTA | 6553 | CB | ASP | | 32 | 13.347 | 64.802 | 23.209 | 1.00 46.83 | | | Ċ |
| | ATOM. | 6556 | CG | ASP | | 32 | | 63.952 | 23.614 | 1.00 57.65 | • | | ō |
| | ATOM | 6557 | | ASP | | 32 | 12.601 14.037 | 64.597 | 22.118 | 1.00 28.18 | | | o. |
| 20 | ATOM | 6558 | | ASP | | 32 | 15.937 | 65.627 | 24.483 | 1.00 50.93 | | | Č |
| 30 | MOTA | 6559 | C | ASP | | 32 | 16.137 | 66.095 | 23.372 | 1.00 56.78 | - | • | ō |
| | MOTA | 6560 | 0 | ASP | | 32 | | 64.901 | 25.091 | 1.00 44.66 | | | N |
| | MOTA | 6561 | N | THR | | 33 33 | 16.854 18.135 | 64.814 | 24.467 | 1.00 41.11 | | | C |
| | ATOM | 6563 | CA | THR | | 33 | 19.151 | 64.207 | 25.419 | 1.00 44.39 | | | C |
| 26 | MOTA | 6565 | CB | THR THR | | 33 | 18.649 | 62.989 | 25.966 | 1.00 47.50 | | • | ō |
| 35 | ATOM | 6567 | | | | 33 | 19.298 | 65.077 | 26.643 | 1.00 45.76 | | | c |
| | ATOM | 6569 | CGZ | THR THR | | 33 . | 18.075 | 64.056 | 23.159 | 1.00 43.39 | | | c |
| | ATOM | 6573 | 0 | THR | | 33 33 | 19.101 | 63.882 | 22.521 | 1.00 45.31 | | | 0 |
| • | MOTA | 6574 6575 | N | GLY | | 34 | 16.891 | 63.610 | 22.749 | 1.00 43.77 | | | N |
| 40 | MOTA | 6577 | CA | GLY | | 34 | 16.739 | 62.822 | 21.528 | 1.00 46.99 | | | С |
| 40 | ATOM | 6580 | C | GLY | | 34 | 16.380 | 63.629 | 20.282 | 1.00 49.16 | | | C |
| | ATOM | 6581 | o | GLY | | 34 | 16.324 | 63.093 | 19.151 | 1.00 50.21 | | | 0 |
| | ATOM ATOM | 6582 | N | SER | | 35 | 16.151 | 64.924 | | 1.00 50.26 | | | N |
| | ATOM | 6584 | CA | SER | | 35 | 15.776 | 65.838 | 19.394 | 1.00 47.28 | | | С |
| 45 | ATOM | 6586 | CB | SER | | 35 | 14.281 | 66.025 | 19.398 | 1.00 43.53 | | | , C |
| 43 | ATOM | 6589 | OG | SER | | 35 | 13.916 | 66.661 | 20.582 | 1.00 41.18 | | | Q |
| | ATOM | 6591 | C. | SER. | | 35 | 16.491 | 67.207 | 19.504 | 1.00 43.05 | | • | С |
| • | ATOM | 6592 | ŏ | SER | | 35 | 17.273 | 67.446 | 20.440 | 1.00 43.12 | | | 0 |
| | ATOM | 6593 | N | SER | | 36 | 16.238 | 68.094 | 18.549 | 1.00 37.14 | | | . N |
| 50 | ATOM . | 6595 | CA | SER | | 36 | 16:982 | 69.332 | 18.512 | 1.00 36.80 | | | С |
| 50 | ATOM | 6597 | CB | SER | | 36 | 18.137 | | | 1.00 40.35 | | | С |
| | ATOM | 6600 | OG | SER | | 36 | 19.229 | 68.365 | 18.021 | 1.00 36.18 | | | 0 |
| | | 6602 | C | SER | | 36 | 16.182 | 70.629 | 18.297 | 1.00 42.36 | | | С |
| | MOTA | 6603 | o | SER | | 36 | 16.739 | 71.718 | 18.339 | 1.00 49.70 | | ÷ | . 0 |
| 55 | MOTA | 6604 | N | ASN | | 37 | 14.879 | 70.560 | 18.107 | 1.00 45.23 | | | N |
| ככ | ATOM | 6606 | - CA | ASN | | 37 | 14.135 | 71.783 | 17.906 | 1.00 44.85 | | | С |
| • | ATOM | 6608 | CB | ASN | | 37 | 13.080 | 71.617 | 16.845 | 1.00 43.43 | | | С |
| | MOTA | 6611 | CG | ASN | | 37 | 13.659 | 71.592 | 15.492 | 1.00 49.01 | | | C |
| | ATOM | 6612 | | ASN | | 37 | 14.303 | | | | | | 0 |
| 60 | ATOM | 6613 | | ASN | | 37 | 13.450 | | 14.715 | | | | N |
| OU | ATOM | 6616 | C | | | 37 | 13.432 | | 19.164 | | | | C |
| | MOTA | 0010 | C | ASN | D | 31 | 10.432 | | 13.104 | 1.00 10.0 | | | • |

| | | | | | | | | | | • | | | | | |
|-----------|--------|-------|-----|-------|-------|-----|-----|------------------|------------------|------------------|------|----------------|---|---|------------|
| 5 | ATOM | 6617 | 0 | ASN I | В | 37 | | 12.955 | 71.279 | 19.843 | | 48.92 | | | 0 |
| | MOTA | 6618 | N | PHE I | B., ' | 38. | - ; | 13.379 | 73.447 | 19.454 | | 39.62 | | | N |
| | MOTA | 6620 | CA | PHE I | В | 38 | • | 12.666 | 73.984 | 20.588 | | 37.09 | | | С |
| | ATOM | 6622 | CB | PHE I | В | 38 | | 13.518 | 75.084 | 21.189 | | 34.12 | , | | С |
| | MOTA | 6625 | CG | PHE 1 | В | 38 | | 12.915 | 75.809 | 22.291 | | 36.88 | | | С |
| 10 | ATOM | 6626 | CD1 | PHE 1 | В. | 38 | | 13.190 | 77.128 | 22.451 | | 43.04 | | | С |
| | ATOM | 6628 | CE1 | PHE I | В | 38 | | 12.639 | 77.847 | 23.480 | | 43.52 | | | С |
| | MOTA | 6630 | CZ | PHE 1 | В | 38 | | 11.810 | 77.261 | 24.366 | | 45.02 | | | С |
| | ATOM | 6632 | | PHE 1 | В | 38 | | 11.519 | 75.950 | 24.235 | | 51.64 | | | С |
| | MOTA | 6634 | CD2 | PHE T | В | 38 | | 12.082 | 75.213 | 23.185 | | 52.30 | | | C |
| 15 | ATOM | 6636 | С | PHE 1 | В | 38 | | 11.313 | 74.445 | 20.010 | | 40.81 | | | С |
| | ATOM | 6637 | 0 | PHE 1 | В | 38 | | 11.241 | 75.206 | 19.018 | | 42.46 | | | 0 |
| | ATOM | 6638 | N | ALA I | В | 39 | | 10.238 | 73.940 | 20.607 | | 40.42 | | | N |
| | MOTA | 6640 | CA | ALA ! | В | 39 | | 8.903 | 74.198 | 20.105 | | 44.90 | | | C . |
| • . | MOTA | 6642 | CB | ALA : | В | 39 | | 8.473 | 73.061 | 19.113 | | 45.36 | | | C |
| 20 | MOTA | 6646 | C | ALA | В | 39 | | 7.889 | 74.308 | 21.212 | | 41.28 | | | С |
| | ATOM | 6647. | 0 | ALA | В | 39 | | 7.961 | 73.617 | 22.213 | | 44.60 | | | 0 |
| | ATOM | 6648 | N | VAL | В | 40 | | 6.929 | 75.177 | 21.046 | | 40.49 | | | N |
| | MOTA | 6650 | CA | VAL | В | 40 | | 5.885 | 75.186 | 22.027 | | 49.83 | | | С |
| | ATOM | 6652 | СВ | VAL | В | 40 | | 6.020 | 76.354 | 22.997 | | 49.55 | • | | С |
| 25 | ATOM | 6654 | CG1 | VAL | В | 40 | | 7.345 | 76.332 | 23.631 | | 46.17 | | | С |
| • | MOTA | 6658 | CG2 | VAL | В | 40 | | 5.830 | 77.657 | 22.280 | | 54.69 | | | С |
| | MOTA | 6662 | С | VAL | В | 40 | | 4.496 | 75.202 | 21.404 | | 51.60 | | | С |
| | ATOM | 6663 | 0 | VAL | В | 40 | | 4.209 | 75.904 | 20.435 | | 56.20 | | | 0 |
| | ATOM | 6664 | N | GLY | В | 41 | | 3.629 | 74.394 | 21.958 | | 50.81 | | | N |
| 30 | ATOM | 6666 | CA. | GLY | В | 41 | | 2.235 | 74.528 | 21.608 | | 54.35 | | | С |
| | MOTA | 6669 | С | GLY | В | 41 | | 1.861 | 76.000 | 21.658 | | 54.27 | | | С |
| | ATOM | 6670 | 0 | GLY | В | 41 | | 2.139 | 76.715 | 22.646 | | 50.40 | | | 0 |
| | MOTA | 6671 | N | ALA | | 42 | | 1.208 | 76.439 | 20.585 | | 55.45 | | | N |
| | MOTA | 6673 | CA | ALA | | 42 | ٠. | 0.864 | 77.840 | 20.394 | | 57.72 | | | C |
| 35 | MOTA | 6675 | CB | ALA | | 42 | | 1.661 | | 19.208 | | 61:49 | | | C |
| | MOTA | 6679 | C | ALA | | 42 | | -0.620 | 78.089 | 20.158 | | 59.93 | | | C |
| | ATOM | 6680 | 0 | ALA | | 42 | | -1.041 | 79.239 | 19.956 | | 54.51 | | | O N |
| | MOTA | 6681 | N | ALA | | 43 | | -1.422 | 77.028 | 20.205 | | 59.25 | | • | C |
| | MOTA | 6683 | CA | ALA | | 43 | | -2.838 | 77.148 | 19.904 | | 58.08 | | | c |
| 40 | MOTA | 6685 | CB | ALA | | 43 | | -3.069 | 76.951 | 18.403 | | 57.09 | | | c |
| | MOTA | 6689 | C | ALA | | 43 | | -3.577 | 76.084 | 20.669 | | 57.28 57.71 | | | ŏ |
| | MOTA | 6690 | 0 | ALA | | 43 | | -3.047 | 75.011 76.358 | 20.869 21.067 | | 58.13 | | | Ŋ |
| | ATOM | 6691 | N | PRO | | 44 | | -4.809 -5.568 | 75.407 | 21.856 | | 55.97 | | | c |
| 4.5 | MOTA | 6692 | CA | PRO | | 44 | | | 75.819 | 21.550 | | 57.92 | | | Č |
| 45 | ATOM | 6694 | CB | PRO | | 44 | | -7.009 | 76.827 | 20.407 | | 57.30 | | • | Č |
| | MOTA | 6697 | CG | PRO | | 44 | | -6.845 -5.628 | 77.554 | 20.804 | • | 57:17 | | | Č |
| | MOTA | 6700 | CD | PRO | | 44 | | | | | | 55.26 | | | Č |
| | MOTA | 6703 | С | PRO | | 44 | | -5.339 | 73.798 | 20.199 | | 55.54 | • | | Ö |
| ~0 | ATOM | 6704 | | PRO | | 44 | | -5.058 | 73.790 | 22.330 | | 51.68 | | | N |
| 50 | ATOM . | 6705 | N | HIS | | 45 | | -5.458 | | 22.074 | | 49.63 | | • | C |
| | ATOM | 6707 | CA | HIS | | 45 | • | -5.380 | 71.662 71.199 | 21.920 | | 47.73 | | | Ċ. |
| | ATOM | 6709 | CB | HIS | | 45 | | -3.960 | 69.743 | 21.624 | | 47.10 | | | Č |
| | ATOM | 6712 | CG | HIS | | 45 | | -3.854 | | 22.613 | | 47.83 | • | | N |
| | ATOM | 6713 | | HIS | | 45 | | -3.661 | 68.805 67.602 | 22.062 | | 48.34 | ' | | C. |
| 55 | ATOM | 6715 | | HIS | | 45 | | -3.628 | | 20.755 | | 39.59 | | | N |
| | ATOM | 6717 | | HIS | | 45 | | -3.798 | 67.728 69.058 | | | 37.38 | | | C |
| | MOTA | 6719 | | HIS | | 45 | | -3.932 | | | | 54.88 | | | č |
| | MOTA | 6721 | C | HIS | | 45 | | -5.990 -5.950 | | | | 61.00 | | | ŏ |
| 60 | MOTA | 6722 | 0 | HIS | | 45 | | -5.850 | | | | 58.61 | | | N |
| 60 | MOTA | 6723 | N | PRO | | 46 | | -6.670 | | | | 58.25 | * | | c |
| | MOTA | 6724 | CA | PRO | B | 46 | | -7.391 | 07.467 | 63.312 | 1.00 | | | | • |
| | | | | | | | | | | | | | | | |

| E . | 3 mOM | c726 | СВ | PRO | p | 46 | | -8.093 | 68.157 | 23.840 | | 56.69 | | | С |
|-------------|-------|--------------|-----|-------|-----|------|---|--------|--------|--------|------|---------|---|---|-----|
| 5 | ATOM | 6726 | | PRO | | 46 | | -8.000 | 68.181 | 22.353 | 1.00 | 55.11 | | | С |
| • | ATOM | 6729 | CG | PRO | | 46 | | -6.815 | 69.046 | 22.032 | 1.00 | 60.22 | | | С |
| | ATOM | 6732 | CD | PRO | | 46 | | -6.491 | 69.075 | 25.575 | 1.00 | 57.99 | | | С |
| | ATOM | 6735 | C | | | 46 | • | -6.953 | 68.992 | 26.716 | 1.00 | 56.13 | | • | 0 |
| | MOTA | 6736 | 0 | PRO | | 47 | | -5.206 | 68.871 | 25.356 | | 55.88 | | | N |
| 10 | MOTA | 6737 | N | PHE | | | | -4.396 | 68.376 | 26.470 | | 51.81 | | | С |
| • | MOTA | 6739 | CA | PHE | | 47 | | | 67.274 | 25.982 | | 44.88 | | | С |
| | MOTA | 6741 | CB | PHE | | 47 | | -3.499 | 66.044 | 25.604 | | 46.77 | | | С |
| | MOTA | 6744 | CG | PHE | | 47 | | -4.234 | 65.093 | 24.782 | | 49.70 | | | С |
| | MOTA | 6745 | | PHE | | 47 | | -3.640 | | 24.702 | 1 00 | 48:35 | | | C |
| 15 | MOTA | 6747 | | PHE | | 47 | | -4.315 | 63.949 | | | 43.45 | | | Č |
| | MOTA | 6749 | CZ | PHE | | | | -5.596 | 63.746 | 24.901 | | 36.92 | | | Č. |
| | MOTA | 6751 | | PHE | | 47 | | -6.205 | | 25.729 | | 43.75 | | | č |
| | MOTA | 6753 | CD2 | PHE | В | 47 | | -5.530 | 65.822 | 26.070 | | 53.07 | | | ç |
| • | MOTA | 6755 | С | PHE | В | 47 | | -3.532 | 69.385 | 27.152 | | | | | Ö |
| 20 | ATOM | 6756 | 0 | PHE | В | 47 | | -2.763 | 69.015 | 28.046 | | 56.38 | | | N |
| | MOTA | 6757 | N | LEU | В | 48 | | -3.661 | 70.647 | 26.760 | | 48.06 | | | |
| | ATOM | 6759 | CA | LEU | В | 48 | | -2.719 | 71.620 | 27.207 | | 49.14 | | | C · |
| | ATOM | 6761 | CB | LEU | В | 48 | | -2.107 | 72.333 | 26.014 | | 50.40 | | | C |
| | MOTA | 6764 | CG | LEU | В | 48 | | -1.214 | 71.667 | 24.990 | | 47.31 | | | C |
| 25 | ATOM | 6766 | CD1 | LEU | В | 48 | | -1.252 | 72.578 | 23.755 | | 47.58 | | | C |
| 23 | MOTA | 6770 | | LEU | | 48 | | 0.179 | 71.567 | 25.528 | | 48.26 | | | С |
| | ATOM | 6774 | C | LEU | | 48 | | -3.453 | 72.636 | 27.955 | | 53.07 | | | С |
| | ATOM | 6775 | ō | LEU | | 48 | | -4.383 | 73.194 | 27.396 | 1.00 | 55.21 | | | 0 |
| | ATOM | 6776 | N | HIS | | 49 | | -3.033 | 72.940 | 29.181 | | 57.93 | | | N |
| 30 | | 6778 | CA | HIS | | 49 | | -3.757 | 73.897 | 30.015 | 1.00 | 56.76 | • | | С |
| 30 | MOTA | 6780 | CB | HIS | | 49 | | -3.451 | 73.706 | 31.497 | 1.00 | 61.80 | | | С |
| | ATOM | | CG | HIS | | 49 | | -4.070 | 72.466 | 32.048 | 1.00 | 67.51 | | | C |
| | ATOM | 6783 6784 | | HIS | | 49 | | -5.274 | 71.984 | 31.583 | 1.00 | 65.77 | | | N. |
| | ATOM | | | HIS | | 49 | | ~5.579 | | 32.226 | 1.00 | 68.88 | | | C |
| 25 | ATOM | 6786 | | HIS | | 49 | | -4.615 | 70.615 | 33.092 | | 72.14 | | | N |
| 35 . | MOTA | 6788 | | HIS | | 49 | | -3.654 | 71.596 | 32.999 | | 70.39 | | | C |
| | MOTA | 6790 | | HIS | | 49 | | -3.484 | 75.276 | 29.617 | | 55.32 | ٠ | | C |
| | ATOM | 6792 | C C | | | 49 | | -4.365 | 76.100 | 29.747 | | 54.19 | | • | 0 |
| | ATOM | 6793 | 0 | HIS | | 50 | | -2.278 | 75.563 | 29.139 | | 57.08 | | | N |
| 40 | ATOM | 6794 | N | ARG | | 50 | | -1.920 | 76.933 | 28.702 | | 52.78 | | | С |
| 40 | ATOM | 6796 | CA | | | 50 | | -1.133 | | 29.796 | | 48.76 | | | C |
| | MOTA | 6798 | CB | ARG | | | | -0.218 | | 30.591 | | 53.36 | | | С |
| · | MOTA | 6801 | CG | ARG | | 50 | | 0.743 | | 31.593 | | 54.71 | | | С |
| | ATOM | 6804 | CD | ARG | | 50 | | | | 31.868 | | 61.19 | | | N |
| | MOTA | 6807 | NE | ARG | | 50 | | 1.853 | | | | 59.08 | | • | С |
| 45 | ATOM | 6809 | CZ | ARG | | 50 | | 2.737 | | | | 60.26 | | | N |
| • | MOTA | 6810 | | ARC | | 50 | | 2.693 | 1 . | | | 66.01 | | | N |
| | ATOM | 6813 | | 2 ARC | | 50 | | 3.681 | | | | 54.68 | | | C |
| | MOTA | 6816 | С | ARC | | 50 | | -1.078 | | | | | | | ŏ |
| | MOTA | 6817 | 0 | ARC | şΒ | | | -0.699 | | | | 57.99 | | | И |
| 50 | ATOM | 6818 | N | TY | R B | | | | 77.896 | | | 55.14 | | | c |
| | ATOM | 6820 | CA | TYI | RВ | | | | 77.836 | | | 51.39 | • | | c. |
| ٠. | ATOM | 6822 | CB | TY | R B | 51 | | -0.692 | | | | 52.11 | | | |
| | MOTA | 6825 | CG | TYI | RВ | 51 | | -1.939 | | | | 50.59 | | | C |
| | MOTA | 6826 | | 1 TY | R B | 51 | | -1.872 | 79.145 | | | 53.23 | | | C |
| 55 | ATOM | 6828 | | 1 TY | | | | -3.007 | | | | 54.06 | | | C |
| | ATOM | 6830 | | | R B | | | -4.238 | | 22.977 | | 56.68 | | | . C |
| | MOTA | 6831 | | | R B | | | -5.428 | | | | 55.76 | | | 0 |
| | | 6833 | | 2 TY | | | | -4.311 | | | 1.00 | 56.57 | | | С |
| | MOTA | 6835 | | 2 TY | | | | -3.178 | | | | 55.59 | | | C |
| 60 | MOTA | 6837 | | | RB | | • | 0.654 | | | | 0 49.19 | | | С |
| .00 | ATOM | | | | RE | | | 0.394 | | | | 0 48.94 | | | 0 |
| | MOTA | 6838 | U | 11 | . E | , ,, | | J.J. | | | | | | | |

| . 5 | ATOM | 6839 | N | TYR | В | 52 | 1.503 | 79.151 | 24.193 | 1.00 47.59 | | | N |
|------|------|------|-----|-------|----|----|--------|--------|--------|------------|---|---|----|
| | ATOM | 6841 | CA | TYR | В. | 52 | 2.182 | 80.378 | 23.852 | 1.00 50.52 | | | С |
| | MOTA | 6843 | CB | TYR | В | 52 | 3.496 | 80.019 | 23.199 | 1.00 44.85 | | | С |
| | MOTA | 6846 | CG | TYR | | 52 | 4.382 | 81.161 | 22.853 | 1.00 43.08 | | | С |
| | MOTA | 6847 | CD1 | TYR | В | 52 | 4.498 | 82.273 | 23.656 | 1.00 45.53 | | | С |
| 10 | MOTA | 6849 | CE1 | TYR | В | 52 | 5.355 | 83.314 | 23.297 | 1.00 43.96 | | | С |
| | ATOM | 6851 | CZ | TYR | В | 52 | 6.080 | 83.202 | 22.134 | 1.00 41.86 | | | С |
| | ATOM | 6852 | ОН | TYR | В | 52 | 6.952 | 84.165 | 21.695 | 1.00 54.44 | | | 0 |
| | ATOM | 6854 | CE2 | TYR | ·B | 52 | 5.969 | 82.123 | 21.357 | 1.00 43.09 | | | С |
| | MOTA | 6856 | CD2 | TYR | В | 52 | 5.138 | 81.113 | 21.705 | 1.00 46.61 | | | С |
| 15 | ATOM | 6858 | С | TYR - | В | 52 | 1.327 | 81.241 | 22.914 | 1.00 53.39 | | | С |
| | MOTA | 6859 | O | TYR | В | 52 | 0.897 | 80.763 | 21.840 | 1.00 55.11 | | | 0 |
| | ATOM | 6860 | N | GLN | В | 53 | 1.066 | 82.488 | 23.312 | 1.00 49.66 | | | N |
| | ATOM | 6862 | CA | GLN | В | 53 | 0.350 | 83.402 | 22.424 | 1.00 53.39 | | | С |
| • | MOTA | 6864 | CB | GLN | В | 53 | -0.928 | 83.978 | 23.029 | 1.00 57.67 | | | С |
| 20 | ATOM | 6867 | CG | GLN | В | 53 | -1.673 | 83.154 | 24.073 | 1.00 58.49 | | | C |
| | ATOM | 6870 | CD. | GLN | В | 53 | -2.674 | 84.056 | 24.766 | 1.00 63.66 | | | С |
| | ATOM | 6871 | OE1 | GLN | В | 53 | -2.341 | 84.707 | 25.784 | 1.00 62.18 | | | 0 |
| | ATOM | 6872 | NE2 | GLN | В | 53 | -3.891 | 84.146 | 24.200 | 1.00 60.51 | • | | N |
| | ATOM | 6875 | С | GLN | | 53 | 1.254 | 84.569 | 21.988 | 1.00 54.38 | | | С |
| 25 | ATOM | 6876 | 0 | GLN | В | 53 | 1.569 | 85.510 | 22.750 | 1.00 49.25 | • | | 0 |
| | ATOM | 6877 | N | ARG | В | 54 | 1.657 | 84.494 | 20.735 | 1.00 50.22 | | | N |
| | ATOM | 6879 | CA | ARG | В | 54 | 2.547 | 85.458 | 20.202 | 1.00 45.95 | | | С |
| | ATOM | 6881 | СВ | ARG | В | 54 | 2.907 | 85.045 | 18.778 | 1.00 45.10 | | | С |
| | ATOM | 6884 | CG | ARG | | 54 | 3.655 | 83.672 | 18.783 | 1.00 39.53 | | | С |
| 30 | ATOM | 6887 | CD | ARG | В | 54 | 3.679 | 82.890 | 17.474 | 1.00 42.75 | | | С |
| | ATOM | 6890 | NE | ARG | В | 54 | 2.387 | 82.353 | 17.079 | 1.00 47.37 | | | N |
| | ATOM | 6892 | CZ | ARG | | 54 | 2.139 | 81.788 | 15.910 | 1.00 45.51 | | | С |
| | ATOM | 6893 | NH1 | ARG | В | 54 | 3.100 | 81.680 | 15.024 | 1.00 51.53 | | | N |
| | ATOM | 6896 | NH2 | ARG | В | 54 | 0.931 | 81.330 | 15.618 | 1.00 42.27 | | | N |
| 35 | ATOM | 6899 | С | ARG | В | 54 | 1.939 | 86.836 | 20.386 | 1.00 52.82 | | • | С |
| | ATOM | 6900 | 0 | ARG | В | 54 | 2.439 | 87.560 | 21.225 | 1.00 59.82 | | | 0 |
| | ATOM | 6901 | N | GLN | | 55 | 0.855 | 87.196 | 19.686 | 1.00 57.85 | | | N |
| | ATOM | 6903 | CA | GLN | В | 55 | 0.303 | 88.572 | 19.736 | 1.00 57.16 | | | С |
| | MOTA | 6905 | CB- | GLN | В | 55 | -1.194 | 88.640 | 19.347 | 1.00 62.44 | | | С |
| 40 | MOTA | 6908 | CG | GLN | В | 55 | -1.469 | 88.563 | 17.810 | 1.00 70.53 | | | С |
| | ATOM | 6911 | CD | GLN | В | 55 | -2.978 | 88.687 | 17.382 | 1.00 79.43 | | | С |
| | ATOM | 6912 | OE1 | GLN | В | 55 | -3.369 | 89.660 | 16.701 | 1.00 80.66 | | | 0 |
| | ATOM | 6913 | NE2 | GLN | В | 55 | -3.802 | 87.692 | 17.764 | 1.00 79.42 | | | N |
| | MOTA | 6916 | С | GLN | В | 55 | 0.533 | 89.312 | 21.058 | 1.00 57.92 | | | С |
| 45 | ATOM | 6917 | 0 | GLN | | 55 | 0.360 | 90.526 | 21.117 | 1.00 56.14 | | | 0 |
| | ATOM | 6918 | N | LEU | | 56 | 0.930 | 88.622 | 22.121 | 1.00 55.89 | | | N |
| | ATOM | 6920 | CA | LEU | В. | 56 | 1.213 | 89.336 | 23.370 | 1.00 58.18 | | | С |
| | ATOM | 6922 | CB | LEU | | 56 | 0.712 | 88.524 | 24.540 | 1.00 60.42 | | | C |
| | ATOM | 6925 | CG | LEU | | 56 | -0.721 | 88.029 | 24.402 | 1.00 62.37 | | | c´ |
| - 50 | ATOM | 6927 | | LEU | | 56 | -1.296 | 87.699 | 25.797 | 1.00 63.41 | | | С |
| | ATOM | 6931 | | LEU | | 56 | -1.598 | 89.054 | 23.676 | 1.00 62.35 | | | С |
| | ATOM | 6935 | С | LEU | | 56 | 2.666 | 89.723 | | 1.00 60.41 | | | С |
| | ATOM | 6936 | 0 | LEU | | 56 | 2.861 | 90.367 | 24.719 | 1.00 60.04 | | | o. |
| | ATOM | 6937 | N | SER | | 57 | 3.663 | 89.348 | 22.857 | 1.00 57.76 | | | N |
| 55 | ATOM | 6939 | CA | SER | | 57 | 5.071 | 89.701 | 23.116 | 1.00 54.64 | | • | C |
| | ATOM | 6941 | СВ | SER | | 57 | 5.991 | 88.475 | 23.117 | 1.00 56.81 | | | c |
| | ATOM | 6944 | OG | SER | | 57 | 7.344 | 88.844 | 23.423 | 1.00 54.08 | | | ō |
| | ATOM | 6946 | C | SER | | 57 | 5.661 | 90.710 | 22.153 | 1.00 53.95 | | | č |
| | ATOM | 6947 | ŏ | SER | | 57 | 5.658 | 90.533 | 20.942 | 1.00 55.46 | | | ō |
| 60 | ATOM | 6948 | N | SER | | 58 | 6.218 | 91.755 | 22.738 | 1.00 53.46 | | | N |
| 00 | ATOM | 6950 | CA | SER | | 58 | | 92.873 | 22.730 | 1.00 32.39 | | | C |
| | AION | 0550 | CA | SEK | D | 20 | 6.736 | 32.013 | 22.011 | 1.00 40.14 | | | C |

| 5 | ATOM | 6952 | CB | SER E | 3 | 58 . | | 6.820 | 94.070 | 22.947 | | 47.29 | | | С |
|------|--------------|------|-----|-------|---|------|---|--------|------------------|--------|------|---------|-----|----|----|
| | ATOM | 6955 | | SER E | | 58 | | 7.567 | 93.825 | 24.116 | | 47.06 | . : | 1. | 0 |
| | ATOM | 6957 | | SER E | | 58 | | 8.114 | 92.536 | 21.420 | 1.00 | 47.84 | | | C, |
| | MOTA | 6958 | - | SER E | | 58 | | 8.576 | 93.177 | 20.478 | 1.00 | 47.48 | | | 0 |
| | MOTA | 6959 | - | THR E | | 59 | | 8.747 | 91.510 | 21.965 | 1.00 | 48.33 | | | N |
| 10 | MOTA | 6961 | | THR E | | 59 | | 10.006 | 91.008 | 21.429 | 1.00 | 42.92 | | | С |
| 10 | ATOM | 6963 | | THR E | | 59 | | 10.885 | 90.549 | 22.559 | 1.00 | 42.65 | | | С |
| | | 6965 | | THR E | | 59 | | 10.128 | 89.795 | 23.523 | 1.00 | 49.24 | | | 0 |
| | ATOM ATOM | 6967 | | THR E | | 59 | | 11.359 | 91.709 | 23.347 | | 45.57 | | | С |
| | | 6971 | C | THR I | | 59 | | 9.812 | 89.853 | 20.405 | | 45.53 | | | C |
| 15 | ATOM | | 0 | THR I | | 59 | | 10.800 | 89.319 | 19.883 | | 42.19 | | | 0 |
| 15 | MOTA | 6972 | | TYR I | | 60 | | 8.566 | 89.465 | 20.113 | | 44.25 | | | N |
| | ATOM | 6973 | N | TYR I | | 60 | • | 8.312 | 88.440 | 19.089 | 1.00 | 42.52 | • | | С |
| | MOTA | 6975 | CA | TYR I | | 60 | | 6.854 | 88.060 | 19.079 | | 42.61 | | | С |
| ٠. | MOTA | 6977 | CB | | | | | 6.444 | 87.188 | 17.912 | | 39.56 | | | С |
| | MOTA | 6980 | CG | TYR I | | 60 | | 6.853 | 85.902 | 17.825 | | 39.91 | | • | C. |
| 20 | MOTA | 6981 | | TYR I | | 60 | | | 85.088 | 16.766 | | 37.80 | | | Č |
| | MOTA | 6983 | | TYR I | | 60 | | 6.478 | 85.576 | 15.787 | | 41.24 | | | c |
| | MOTA | 6985 | CZ | TYR I | | 60 | | 5.693 | | 14.726 | | 49.70 | | | ō |
| | MOTA | 6986 | OH | TYR ! | | 60 | | 5.341 | 84.743 | 15.855 | | 38.20 | | | Ċ |
| | MOTA | 6988 | | TYR I | | 60 | | 5.263 | 86.875 87.661 | 16.909 | | 40.65 | | | Č |
| 25 | MOTA | 6990 | CD2 | TYR | | 60 | | 5.636 | | 17.691 | | 47.70 | • | | Ċ |
| | MOTA | 6992 | С | TYR | | 60 | | 8.593 | 88.944 | | | 45.23 | | | ő |
| | ATOM | 6993 | 0 | TYR | | 60 | | 8.100 | 89.986 | 17:310 | | 53.11 | | | N |
| | MOTA | 6994 | N | ARG : | | 61 | | 9.376 | 88.195 | 16.913 | | 47.96 | | | C |
| | ATOM | 6996 | CA | ARG | | 61 | | 9.536 | 88.482 | 15.488 | | 48.51 | | | Č |
| 30 | ATOM | 6998 | CB | ARG | | 61 | | 10.866 | 89.084 | 15.173 | | 47.51 | | | Č |
| | MOTA | 7001 | CG | ARG | | 61 | | 11.328 | 90.014 | 16.186 | | | | | Č |
| | MOTA | 7004 | CD | ARG | | 61 | | 12.777 | 90.163 | 16.129 | | 46.49 | | | N |
| | MOTA | 7007 | NE | ARG | | 61 | | 13.175 | 91.480 | 16.568 | | 53.97 | | | C |
| | ATOM | 7009 | CZ | ARG | | 61 | | 14.425 | 91.808 | 16.746 | | 57.00 | | | N |
| : 35 | MOTA | 7010 | | ARG | | 61 | | 15.338 | 90.893 | 16.529 | | 62.31 | | | N |
| | MOTA | 7013 | NH2 | ARG | | 61 | | 14.778 | 93.015 | 17.141 | | 55.13 | | | C |
| | MOTA | 7016 | С | ARG | | 61 | | 9.346 | 87.181 | 14.730 | | 48.27 | | | 0 |
| | MOTA | 7017 | 0 | ARG | | 61 | | 9.609 | 86.115 | 15.238 | | 52.99 | | | N |
| | MOTA | 7018 | N | ASP | | 62 | | 8.910 | 87.304 | 13.496 | | 44.77 | | | |
| 40 | ATOM | 7020 | CA | ASP | | 62 | | 8.336 | 86.217 | 12.776 | | 46.62 | | | C |
| | MOTA | 7022 | CB | ASP | | 62 | | 6.934 | 86.722 | 12.384 | | 49.17 | | | C |
| | ATOM | 7025 | CG | ASP | | 62 | | 6.177 | 85.815 | 11.468 | | 53.87 | | | С |
| | ATOM | 7026 | | ASP | | 62 | | 6.754 | 84.805 | 11.004 | | 55.89 | | | 0 |
| | MOTA | 7027 | OD2 | ASP | В | 62 | | 4.965 | 86.076 | 11.152 | | 54.79 | | | 0 |
| 45 | MOTA | 7028 | С | ASP | В | 62 | | 9.225 | 85.892 | 11.608 | | 49.58 | | | C |
| | MOTA | 7029 | 0 | ASP. | В | 62 | | 9.620 | 86.763 | 10.849 | | 55.62 | | | 0 |
| | MOTA | 7030 | N | LEU | В | 63 | | 9.559 | 84.624 | 11.453 | | 45.53 | | | N |
| | ATOM | 7032 | CA | LEU | В | 63 | | 10.464 | 84.255 | 10.394 | | 42.20 | | | C |
| | MOTA | 7034 | CB | LEU | В | 63 | | 11.360 | 83.083 | 10.835 | | 41.42 | | | C |
| 50 | MOTA | 7037 | CG | LEU | В | 63 | • | 12.548 | 83.387 | 11.771 | | 34.55 | | | С |
| | ATOM | 7039 | CD1 | LEU | В | 63 | | 12.847 | 82.271 | 12.775 | | 36.00 | | | С |
| | ATOM | 7043 | | LEU | | 63 | | 13.742 | 83.634 | 10.972 | | 36.18 | | | С |
| | ATOM | 7047 | C | LEU. | | 63 | | | 83.913 | 9.112 | | 45.11 | | | С |
| | ATOM | 7048 | Ō | LEU | | 63 | · | 10.388 | 83.773 | 8.099 | 1.00 | 51.74 | | | 0 |
| 55 | ATOM | 7049 | N | ARG | | 64 | | 8.407 | 83.778 | 9.132 | 1.00 | 45.09 | | | N |
| 33 | MOTA | 7051 | CA | ARG | | .64 | | 7.627 | 83.437 | 7.918 | | 45.81 | | | C |
| | | 7053 | CB | ARG | | 64 | | 7.621 | 84.590 | 6.932 | | 42.03 | | | С |
| | MOTA | 7056 | CG | ARG | | 64 | | 8.317 | | 7.448 | | 48.52 | | | С |
| • | MOTA | | CD | ARG | | 64 | | 7.647 | | | | 2.44 | | | С |
| 60 | MOTA | 7059 | NE | ARG | | 64 | | | | 5.832 | | 3 45.11 | | | N. |
| 60 | ATOM | 7062 | CZ | ARG | | 64 | • | 9.098 | 88.601 | | | 0 47.61 | ٠ | | С |
| | ATOM | 7064 | C4 | ANG | ט | 04 | | 9.090 | UU. UUI | | | | | | |

| 5 | MOTA | 7065 | NH1. | ARG E | 3 64 | 9.75 | 89.057 | 6.786 | 1.00 | 49.17 | | | N |
|---------------|------|------|------------|-------|-------|-------|---------------|--------|------|-------|---|---|------------|
| _ | MOTA | 7068 | | ARG E | | 9.43 | 89.044 | 4.531 | | | | | N |
| | MOTA | 7071 | С | ARG E | | 8.10 | 82.208 | 7.176 | 1.00 | 48.40 | | | C |
| | ATOM | 7072 | 0 | ARG F | 3 64 | 8.6 | 82.321 | 6.041 | | 50.59 | | | 0 |
| | ATOM | 7073 | N | LYS E | 65 | 8.09 | 81.058 | 7.832 | | 44.70 | | | N |
| 10 | MOTA | 7075 | CA | LYS E | 3 65 | 8.5 | 39 79.783 | 7.378 | 1.00 | 42.44 | | | С |
| | ATOM | 7077 | CB | LYS E | 3 65 | 10.1 | LO 79.799 | 7.680 | | 42.17 | | | С |
| • | ATOM | 7080 | CG | LYS E | | 11.0 | 30 78.794 | 6.970 | | 46.99 | | | С |
| | MOTA | 7083 | CD | LYS E | | 12.5 | | 7.710 | 1.00 | 41.67 | | | . C |
| | ATOM | 7086 | CE | LYS E | | 13.20 | 07 80.010 | 8.378 | 1.00 | 31.79 | | | С |
| 15 | MOTA | 7089 | NZ | LYS E | | 14.6 | 90 79.980 | 8.772 | | 2.00 | | | N |
| | ATOM | 7093 | C . | LYS E | 3 65 | 7.8 | 17 78.802 | 8.271 | 1.00 | 40.97 | • | | С |
| | ATOM | | o | LYS E | | 7.6 | 79.069 | 9.459 | | 39.90 | | • | 0 |
| | ATOM | 7095 | N | GLY E | | 7.2 | 99 77.707 | 7.711 | 1.00 | 45.11 | | | N |
| • | ATOM | 7097 | CA | GLY F | | 6.6 | 32 76.656 | 8.487 | 1.00 | 37.19 | | | С |
| 20 | ATOM | 7100 | С | GLY E | | 7.6 | 43 75.541 | 8.684 | 1.00 | 43.52 | | | С |
| -, | ATOM | 7101 | O | GLY E | | 8.6 | 38, 75.469 | 7.970 | 1.00 | 43.64 | : | | 0 |
| | ATOM | 7102 | N | VAL E | B 67 | 7.3 | 98 . 74 . 674 | 9.652 | | 48.15 | | | N |
| | ATOM | 7104 | CA | VAL I | B 67 | 8.3 | 00 73.575 | 9.969 | 1.00 | 47.91 | | | С |
| | ATOM | 7106 | СВ | VAL E | B 67 | 9.3 | 47 74.093 | 10.970 | 1.00 | 46.06 | | | С |
| 25 | ATOM | 7108 | | VAL E | | 8.6 | 84 74.740 | 12.148 | 1.00 | 53.01 | | | C |
| | ATOM | 7112 | | VAL I | | 10.2 | | 11.460 | | 45.35 | | | С |
| | ATOM | 7116 | c | VAL I | B 67 | 7.5 | 31 72.375 | 10.546 | | 48.93 | | | С |
| | ATOM | 7117 | 0 | VAL I | | 6.6 | | 11.306 | 1.00 | 50.43 | | | . 0 |
| | ATOM | 7118 | N | TYR I | | 7.9 | | 10.173 | 1.00 | 54.33 | | | N |
| 30 | MOTA | 7120 | CA | TYR I | B 68 | 7.3 | 07 69.912 | 10.681 | 1.00 | 54.23 | | | C |
| - | ATOM | 7122 | СВ | TYR I | в 68 | . 6.6 | 74 69.180 | 9.496 | 1.00 | 58.61 | | • | С |
| | ATOM | 7125 | CG | TYR I | в 68 | 6.1 | 94 67.743 | 9.740 | 1.00 | 62.41 | | | C |
| | ATOM | 7126 | CD1 | TYR I | в 68 | 5.1 | 51 67.465 | 10.624 | | 65.98 | | | C . |
| | MOTA | 7128 | CE1 | TYR I | B 68 | 4.7 | 09 66.183 | 10.833 | 1.00 | 65.58 | | | С |
| 35 | MOTA | 7130 | CZ | TYR I | B 68 | 5.3 | 03 65.145 | 10.156 | | 70.65 | | | С |
| | MOTA | 7131 | OH | TYR I | B 68 | 4.8 | 74 63.855 | 10.350 | 1.00 | 76.70 | | | 0 |
| | MOTA | 7133 | CE2 | TYR I | в 68 | 6.3 | 30 65.379 | 9.274 | 1.00 | 68.48 | | | С |
| | ATOM | 7135 | CD2 | TYR ! | B 68 | 6.7 | 66 66.677 | 9.067 | | 68.01 | | | С |
| | MOTA | 7137 | C | TYR I | в 68 | 8.3 | 54 68.969 | | | 52.15 | | | С |
| 40 | MOTA | 7138 | 0 | TYR I | B 68 | 9.4 | 46 68.840 | | | 51.11 | | | 0 |
| | ATOM | 7139 | N | VAL | В 69 | 8.0 | 28 68.308 | 12.407 | | 48.81 | | | N |
| | ATOM | 7141 | CA | VAL | в 69 | 8,9 | 31 67.350 | 13.043 | | 41.24 | | | С |
| • | MOTA | 7143 | CB | VAL I | B 69 | 9.4 | 33 67.888 | | | 46.72 | | | С |
| | ATOM | 7145 | CG1 | VAL | в 69 | 10.5 | | 14.976 | | 50.12 | | | С |
| 45 | MOTA | 7149 | CG2 | VAL : | | 9.9 | | 14.276 | | 44.49 | • | | C |
| | ATOM | 7153 | С | VAL : | 4.3 | 8.2 | | 13.454 | | 42.06 | | | . C |
| | MOTA | 7154 | 0 | VAL | | 7.4 | 27 66.130 | 14.335 | | 49.53 | | • | 0 |
| | MOTA | 7155 | N | PRO | в 70 | 8.5 | | | | 44.13 | | | Ŋ |
| | ATOM | 7156 | CA | PRO | в 70 | | | | | | | | C |
| 50 | MOTA | 7158 | CB | PRO | B 70 | | | | | 42.89 | | | С |
| | ATOM | 7161 | CG | PRO | в 70 | | | | | 41.09 | | | C |
| | ATOM | 7164 | CD | PRO | B 70 | | | | | 47.61 | | | C |
| | MOTA | 7167 | C | PRO- | B 70 | | | | | 49.11 | | | . С |
| | ATOM | 7168 | 0 | PRO | B 70 | 10.3 | | | | 49.67 | | | 0 |
| 55 | ATOM | 7169 | N | TYR | | | | | | 50.47 | | | · N |
| • | ATOM | 7171 | CA | TYR | | | | | | 53.44 | | | C |
| | MOTA | 7173 | CB | TYR | | | | | | 53.95 | | | C |
| | MOTA | 7176 | CG | TYR | B 71 | | | | | 54.07 | | | C |
| | MOTA | 7177 | | TYR | | | | | | 54.07 | | | C |
| 60 | MOTA | 7179 | CE1 | TYR | B 71 | 10.4 | | | | 54.76 | | | C |
| | MOTA | 7181 | CZ | TYR | B '71 | 9.4 | 175 65.989 | 18.322 | 1.00 | 49.10 | | | С |
| | | | | | | | | | | | | | |

| • | 7 MON4 | 7102 | ОН | TYR | В. | 71 | | 9.564 | 67.326 | 18.547 | 1.00 49.20 | | | 0 |
|-----|--------|--------------|----|------|-------|--------------|---|--------|--------|--------|------------|---|---|-----|
| 5 | MOTA | 7182 7184 | | TYR | | 71 | | 8.397 | 65.494 | 17.673 | 1.00 52.91 | | | С |
| • | MOTA | 7186 | | TYR | | 71 | | 8.299 | 64.135 | 17.437 | 1.00 55.62 | | | С |
| | ATOM | 7188 | C | TYR | | 71 | | 9.220 | 59.920 | 15.888 | 1.00 57.24 | | | С |
| | MOTA | 7189 | 0 | TYR | | 71 | | 8.666 | 59.564 | 14.848 | 1.00 61.01 | | | 0 |
| 10 | MOTA | | N | THR | | 72 | • | 9.633 | 59.045 | 16.816 | 1.00 56.65 | | | N |
| 10 | MOTA | 7190 | CA | THR | | 72 | | 9.338 | 57.601 | 16.757 | 1.00 49.69 | | | С |
| | MOTA | 7192 | CB | THR | | 72 | | 10.143 | 56.812 | 17.843 | 1.00 45.99 | | | С |
| | MOTA | 7194 | | THR | | 72 | | 11.515 | 56.708 | 17.485 | 1.00 41.99 | | • | 0 |
| | MOTA | 7196 | | THR | | 72 | | 9.736 | 55.355 | 17.907 | 1.00 48.51 | | | С |
| | MOTA | 7198 | | THR | | 72 | | 7.843 | 57.406 | 17.025 | 1.00 51.02 | | | С |
| 15 | MOTA | 7202 | C | THR | | 72 | | 7,208 | 56.549 | 16.431 | 1.00 52.84 | | | 0 |
| | MOTA | 7203 | 0 | GLN | | 73 | | 7.303 | 58.198 | 17.946 | 1.00 48.27 | | | N |
| | ATOM | 7204 | N | GLN | | 73 | • | 5.875 | 58.203 | 18.263 | 1.00 48.31 | | | C |
| | MOTA | 7206 | CA | | | 73 | | | 57.409 | 19.545 | 1.00 51.35 | | | С |
| 0.0 | MOTA | 7208 | CB | GLN | | 73 73 | | 5.749 | 55.888 | 19.423 | 1.00 56.02 | • | | С |
| 20 | ATOM | .7211 | CG | GLN | | 73 | • | 4.857 | 55.255 | 18.344 | 1.00 61.90 | • | | С |
| | MOTA | 7214 | CD | GLN | | 73 | • | 3.792 | 55.792 | 18.018 | 1.00 68.29 | • | | 0 |
| | MOTA | 7215 | | GLN | | 73 73 | | 5.295 | 54.124 | 17.783 | 1.00 62.95 | | | N |
| | MOTA | 7216 | | GLN | | | | 5.437 | 59.654 | 18.470 | 1.00 49.42 | | | С |
| | MOTA | 7219 | С | GLN | | 73 73 | | 5.747 | 60.278 | 19.508 | 1.00 46.54 | | | 0 |
| 25 | MOTA | 7220 | 0 | GLN | | 74 | | 4.722 | 60.214 | 17.499 | 1.00 48.91 | | | N |
| | MOTA | 7221 | N | GLY | | 74 | | 4.305 | 61.606 | 17.608 | 1.00 49.47 | | | С |
| | ATOM | 7223 | ÇA | GLY | | 74 | | 4.933 | 62.541 | 16.584 | 1.00 50.49 | | | C |
| | MOTA | 7226 | С | GLY | | | | 5.998 | 62.255 | 16.005 | 1.00 50.02 | | | 0. |
| | MOTA | 7227 | 0 | GLY | | 74 75 | | 4.266 | 63.674 | 16.375 | 1.00 50.53 | | • | N |
| 30 | MOTA | 7228 | N | LYS | | | | 4.660 | 64.627 | 15.342 | 1.00 52.28 | | | С |
| | MOTA | 7230 | CA | LYS | | 75 | | 4.490 | 63.974 | 13.978 | 1.00 54.30 | | | С |
| | ATOM | 7232 | CB | LYS | | 75 | | 3.047 | 63.970 | 13.545 | 1.00 57.04 | | | С |
| | MOTA | 7235 | CG | LYS | | 75 75 | | 2.877 | 63.711 | 12.065 | 1.00 62.75 | | | С |
| | MOTA | 7238 | CD | LYS | | 75 | | 3.286 | 62.309 | 11.659 | 1.00 69.74 | | | С |
| 35 | MOTA | 7241 | CE | LYS | | 75 | | 3.245 | 62.144 | 10.151 | 1.00 75.75 | | | N |
| | MOTA | 7244 | NZ | LYS | | 75 | | 3.767 | 65.863 | 15.374 | 1.00 48.92 | | | ,C |
| | MOTA | 7248 | C | LYS | | 75 | | 2.624 | 65.773 | | 1.00 50.04 | | | 0 |
| | MOTA | 7249 | 0 | | 3 B | 75 | | 4.288 | 67.005 | 14.939 | 1.00 47.21 | | | N |
| | MOTA | 7250 | N | | P B | 76 | | 3.529 | 68.264 | 14.876 | 1.00 45.93 | | | С |
| 40 | MOTA | 7252 | CA | | P B | 76 | | 3.623 | 69.023 | 16.212 | 1.00 44.91 | | | С |
| | MOTA | 7254 | CB | | P B | 76 | | 5.006 | 69.104 | | 1.00 44.21 | | | С |
| | MOTA | 7257 | CG | | РВ | 76 | | 5.635 | 68.312 | 17.578 | 1.00 48.52 | | | С |
| | MOTA | 7258 | | 1 TR | | 76 | | 6.950 | 68.697 | 17.720 | 1.00 44.12 | | | N |
| | MOTA | 7260 | | 1 TR | | 76 | | 7.190 | 69.744 | 16.878 | 1.00 40.53 | | | C |
| 45 | MOTA | 7262 | | 2 TR | | 76 | | 5.985 | | | 1.00 46.96 | | • | С |
| | MOTA | 7263 | | 2 TR | | | | 5.967 | 71.072 | | • | | | C. |
| | ATOM | 7264 | | 3 TR | | | | 7.090 | | | 1.00 33.58 | | | С |
| | MOTA | 7266 | | 3 TR | | | | | | | | | | C |
| | MOTA | 7268 | | 2 TR | | | | 8.269 | | | | | | С |
| 50 | MOTA | 7270 | | 2 TR | | | | 8.324 | | | | | | -C |
| | MOTA | 7272 | С | | P B | | | 4.014 | | | | | | 0 |
| | MOTA | 7273 | | | P B | | | 5.038 | | | • | | | . N |
| | MOTA | 7274 | | | U B | | | 3.263 | | | | | • | С |
| | ATOM | 7276 | | | UB | | | 3.588 | | | | | | c |
| 55 | MOTA | 7278 | | | UB | | | 2.687 | | | | | | Ċ |
| | MOTA | 7281 | | | UB | | | 2.928 | | | | | | c |
| | MOTA | 7284 | | | O E | | | 3.069 | | | | | | o |
| | MOTA | 7285 | | 1 GL | | | | 2.692 | | | | | | ő |
| | MOTA | 7286 | | 2 GI | | | | 3.577 | | | 1.00 68.89 | | | C |
| 60 | ATOM | 7287 | | | 'nUE | | | 3.390 | | | | | | o |
| | ATOM | 7288 | 0 | GI | 'nU E | 3 7 7 | ' | 2.470 | 72.671 | 14.038 | 1.00 50.80 | | | J |
| • | | | | | | | | | | | | | | |

| 5 | MOTA | 7289 | N | GLY I | | 78 | 4. | 249 | 73.495 | 12.906 | 1.00 | | | | N |
|------------|------|-------|-----|-------|---|----|-------|-------|---------|--------|------|-------|---|-----|-----|
| | MOTA | 7291 | CA | GLY I | 3 | 78 | - | 116 | 74.794 | 13.527 | | 38.17 | | • • | C |
| | MOTA | 7294 | С | GLY I | В | 78 | 4 . ! | 560 | 75.872 | 12.574 | | 41.86 | | | С |
| | ATOM | 7295 | 0 | GLY I | В | 78 | 4. | 622 | 75.629 | 11.360 | 1.00 | | | | 0 |
| | MOTA | 7296 | N | GLU I | В | 79 | 4. | 865 | 77.040 | 13.150 | | 40.98 | • | | N |
| 10 | MOTA | 7298 | CA | GLU 1 | В | 79 | 5. | 353 | 78.217 | 12.458 | | 40.07 | | | С |
| | MOTA | 7300 | CB | GLU I | В | 79 | 4. | 182 | 79.179 | 12.341 | | 45.01 | | | C. |
| | ATOM | 7303 | CG | GLU I | В | 79 | 3. | 271 | 78.881 | 11.161 | | 48.35 | | | С |
| | ATOM | 7306 | CD | GLU I | В | 79 | 1. | 879 | 79.445 | 11.376 | | 59.96 | | | С |
| | ATOM | 7307 | OE1 | GLU 1 | В | 79 | 1. | 026 | 79.356 | 10.435 | | 58.74 | | | . 0 |
| 15 | ATOM | 7308 | | GLU 1 | | 79 | 1. | 656 | 79.975 | 12.506 | | 62.96 | | | 0 |
| , | ATOM | 7309 | С | GLU I | | 79 | 6. | 534 | 78.904 | 13.206 | | 39.29 | | | С |
| | ATOM | 7310 | 0 | GLU I | В | 79 | 6. | 387 | 79.304 | 14.373 | | 42.71 | | | 0 |
| | ATOM | 7311 | N | LEU I | В | 80 | · 7. | 685 | 79.057 | 12.520 | | 40.28 | | | N |
| • | ATOM | 7313 | CA | LEU ! | | 80 | 8. | 955 | 79.568 | 13.102 | | 36.41 | | | С |
| 20 | ATOM | 7315 | СВ | LEU | | 80 | 10. | 154 | 79.219 | 12.177 | | 36.64 | | | С |
| 20 | ATOM | 7318 | CG | LEU | | 80 | 10. | 738 | 77.781 | 12.076 | 1.00 | 37.91 | | | С |
| | ATOM | 7320 | | LEU | | 80 | 11. | | 77.548 | 10.745 | | 39.77 | | | С |
| | ATOM | 7324 | | LEU | | 80 | | 649 | 77.344 | 13.193 | 1.00 | 36.07 | | | С |
| | ATOM | 7328 | С | LEU | | 80 | | 966 | 81.088 | 13.467 | 1.00 | 33.54 | | | С |
| 25 | ATOM | 7329 | ŏ | LEU | | 80 | | 254 | 81.878 | 12.905 | 1.00 | 32.98 | | | 0 |
| 23 | ATOM | 7330 | N | GLY | | 81 | | 775 | 81.482 | 14.431 | 1.00 | 32.51 | | | N |
| | ATOM | 7332 | CA | GLY | | 81 | | 853 | 82.869 | 14.860 | 1.00 | 36.03 | | | С |
| • | ATOM | 7335 | C | GLY | | 81 | | 029 | 82.934 | 15.848 | 1.00 | 42.04 | | | С |
| | ATOM | 7336 | Ö | GLY | | 81 | | 757 | 81.938 | 15.970 | 1.00 | 29.06 | | | 0 |
| 30 | ATOM | 7337 | N | THR | | 82 | | 223 | 84.089 | 16.504 | 1.00 | 41.12 | | | N |
| 50 | ATOM | 7339 | CA | THR | | 82 | | 122 | 84.225 | 17.659 | 1.00 | 44.53 | | | C |
| • | ATOM | 7341 | CB | THR | | 82 | | 486 | 84.776 | 17.289 | 1.00 | 41.56 | | | С |
| | ATOM | 7343 | | THR | | 82 | | 438 | 86.212 | 17.236 | 1.00 | 37.05 | | | 0 |
| | ATOM | 7345 | | THR | | 82 | • | 898 | 84.298 | 15.882 | 1.00 | 44.94 | | | C |
| 35 | ATOM | 7349 | C | THR | | 82 | | 512 | 85.157 | 18.726 | 1.00 | 47.70 | | | С |
| رر | ATOM | 7350 | Ö | THR | | 82 | | 689 | 86.007 | 18.424 | 1.00 | 48.47 | | | 0 |
| | ATOM | 7351 | N | ASP | | 83 | | 949 | 84.980 | 19.971 | 1.00 | 49.65 | | | N |
| | ATOM | 7353 | CA | ASP | | 83 | | 536 | 85.805 | 21.078 | 1.00 | 43.80 | | | С |
| | ATOM | 7355 | СВ | ASP | | 83 | | .137 | 85.412 | 21.497 | 1.00 | 45.31 | | | С |
| 40 | MOTA | 7358 | CG | ASP | | 83 | | 416 | 86.517 | 22.208 | 1.00 | 48.10 | | | С |
| 4.0 | ATOM | 7359 | | ASP | | 83 | | .063 | 87.357 | 22.873 | 1.00 | 43.35 | | | 0 |
| | ATOM | 7360 | | ASP | | 83 | | .174 | 86.617 | 22.144 | 1.00 | 55.68 | | | 0 |
| | ATOM | 7361 | C | ASP | | 83 | | .515 | 85.545 | 22.220 | 1.00 | 44.30 | | | С |
| | ATOM | 7362 | Ö | ASP | | 83 | | .317 | 84.618 | 22.164 | 1.00 | 42.87 | | | 0 |
| 45 | ATOM | 7363 | N | LEU | | 84 | | .431 | 86.359 | 23.264 | 1.00 | 44.69 | | | N |
| 45 | ATOM | 7365 | CA | LEU | | 84 | | .305 | 86.237 | 24.412 | 1.00 | 44.31 | | | С |
| | ATOM | 7367 | CB | LEU | | 84 | | .298 | 87.556 | 25.184 | 1.00 | 42.41 | | | С |
| | ATOM | 7370 | CG | LEU | | 84 | | .000 | | | 1.00 | 46.49 | | | С |
| | ATOM | 7372 | | LEU | | 84 | | .187 | 89.925 | 25.584 | | 45.21 | | | C |
| 50 | MOTA | 737.6 | | LEU | | 84 | | .355 | 88.390 | 23.988 | | 47.47 | | | C |
| 50 | MOTA | 7380 | C | LEU | | 84 | | .880 | 85.069 | 25.317 | | 43.92 | | | C |
| | ATOM | 7381 | ŏ | LEU | | 84 | | .702 | 84.796 | 25.459 | | 43.23 | • | | 0 |
| | | 7382 | N | VAL | | 85 | | .859 | | 25.939 | | 48.76 | | | N |
| | ATOM | | CA | VAL | | 85 | | .639 | | 26.747 | | 48.52 | | | С |
| 55 | MOTA | 7384 | CB | VAL | | 85 | | .957 | 81.977 | 25.854 | | 49.65 | | | С |
| 55 | ATOM | 7386 | | VAL J | | 85 | | .559 | 80.668 | 26.519 | | 54.85 | | | C |
| | ATOM | 7388 | | VAL | | 85 | | .231 | 82.099 | 24.546 | | 45.28 | | | C |
| | ATOM | 7392 | C | VAL | | 85 | | .484 | 83.123 | 28.044 | | 48.30 | | | С |
| | MOTA | 7396 | o | VAL | | | | .712 | 83.170 | | | 45.59 | | | 0 |
| <i>د</i> ۸ | MOTA | 7397 | | SER | | 86 | | .825 | 83.000 | | | 49.13 | | | N |
| 60 | ATOM | 7398 | N | SER | | 86 | | .515 | 82.778 | | | 50.27 | | | C |
| | MOTA | 7400 | CA | שבת | ם | 00 | 14 | . 713 | 02.1.10 | 5057 | 00 | | | | _ |

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| - | MOTA | 7751 | CG | PHE B | 109 | - | 0.729 | 68.284 | 22.858 | 1.00 44.87 | | | С |
| | MOTA | 7752 | CD1 | PHE B | 109 | | -0.031 | 68.687 | 21.773 | 1.00 47.55 | | | С |
| | MOTA | 7754 | CE1 | PHE B | 109 | | 0.373 | 69.771 | 20.978 | 1.00 46.68 | | | С |
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| 10 | ATOM | 7758 | | PHE B | | | 2.319 | 70.019 | 22.352 | 1.00 46.41 | | | С |
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| | MOTA | 7763 | - | PHE B | | | 0.386 | | | 1.00 57.18 | | | N |
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| • | MOTA | 7773 | CD1 | ILE B | 110 | | 3.487 | 61.911 | 26.109 | 1.00 60.39 | | | С |
| 20 | MOTA | 7777 | CG2 | ILE B | 110 | | 0.839 | 61.703 | 27.968 | 1.00 62.33 | | | C |
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| 25 | | 7787 | CB | GLN E | | | -3.941 | 62.742 | 28.513 | 1.00 66.79 | | | С |
| 25 | ATOM | | | | | | -5.248 | 63.200 | 29.097 | 1.00 70.55 | | | C |
| | ATOM. | 7790 | CG | GLN E | | | | 62.229 | 28.697 | 1.00 72.04 | | | C |
| , | ATOM | 7793 | CD | GLN E | | | -6.356 | | | 1.00 72.04 | | | ŏ |
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| | ATOM | 7799 | 0 | GLN E | | | -1.659 | 62.542 | 30.546 | 1.00 65.83 | | | 0 |
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| | ATOM | 7805 | С | GLY E | 3 112 | | -0.336 | 65.050 | 32.368 | 1.00 65.65 | | | С |
| 35 | ATOM | 7806 | 0 | GLY F | | | 0.120 | 65.257 | 33.492 | 1.00 68.14 | | | 0 |
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| | ATOM | 7831 | Ο. | ASN I | B 114 | | 3.077 | 70.715 | | 1.00 47.48 | | | 0 |
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                                      15.530
             7910
                  CD2 LEU B 119
     MOTA
                                   14.367
                                                                                     C
                                                               1.00 38.35
                                               70.537
                                                       24.053
                      LEU B 119
     ATOM
             7914
                  С
                                                                                    . 0
                                      14.783
                                               69.813
                                                       24.919
                                                               1.00 43.76
                       LEU B 119
35
             7915
                  0
     MOTA
                                                                                     N
                                                               1.00 40.04
                                      14.670
                                               70.384
                                                       22.787
                       GLY B 120
             7916
                  N
     MOTA
                                                               1.00 39.07
                                                                                     C
                                                       22.383
                                      15.509
                                               69.293
                      GLY B 120
     ATOM
             7918
                  ÇA
                                                               1.00 40.82
                                               69.824
                                                       22.631
                       GLY B 120
                                      16.882
            7921
                  С
     MOTA
                                                       22.343
                                                               1.00 40.62
                                      17.085
                                               71.007
                       GLY B 120
             7922
                  0
     MOTA
                                                                                     N
                                                               1.00 35.37
                                      17.802
                                               68.996
                                                       23.150
                       LEU B 121
40
     MOTA
             7923
                  N
                                     19.142
                                                       23.439
                                                               1.00 33.34
                                               69.463
                       LEU B 121
             7925
                  CA
     ATOM
                                                                                     C
                                     19.468
                                                               1.00 34.88
                       LEU B 121
                                               69.229
                                                       24.895
                  CB
     ATOM
             7927
                                                                                     С
                                                               1.00 41.96
                                                       25.920
                       LEU B 121
                                      18.605
                                               69.997
                  CG
     ATOM
             7930
                                                                                     . C
                                                       27.155
                                                               1.00 38.40
                                      18.186
                  CD1 LEU B 121
                                               69.169
             7932
     ATOM
                                                       26.382
                                                               1.00 41.64
                                                                                     С
                                      19.280
                                               71.249
                   CD2 LEU B 121
45
             7936
     ATOM
                                                                                     C
                                                               1.00 38.26
                                      20.169
                                               68.759
                                                       22.554
                       LEU B 121
     ATOM
             7940
                   С
                                                       22.820
                                                                                      0
                                                               1.00 37.48
                                      21.348
                                               68.835
                       LEU B 121
     MOTA
             7941
                   0
                                                                                      N
                                      19.740
                                                       21.489
                                                               1.00 40.79
                                               68.086
                       ALA B 122
     MOTA
             7942
                   N
                                                                                      C
                                                               1.00 42.59
                       ALA B 122
                                   20.697
                                               67.353
                                                       20.674
     ATOM
             7944
                   CA
                                                               1.00 49.22
                                                       19.949
                                   20.045
                                               66.267
                       ALA B 122
50
     ATOM
             7946
                   CB
                                                       19.728
                                                               1.00 45.18
                       ALA B 122
                                     21.322
                                               68.323
             7950
                   С
     ATOM
                                                       19.938
                                                               1.00 45.85
                                               69.515
                       ALA B 122
                                     21.205
             7951
     MOTA
                   0
                                               67.848
                                                       18.697
                                                               1.00 47.39
                       TYR B 123
                                     22.006
             7952
                   N
      MOTA
                                                               1.00 48.54
                                                       17.870
                       TYR B 123
                                       22.763
                                               68.790
             7954
                   CA
      MOTA
                                               68.208
                                                                1.00 50.84
                                                       17.447
                       TYR B 123
                                       24.118
             7956
55
      ATOM
                   CB
                       TYR B 123
                                       25.038
                                               67..830
                                                       18.578
                                                                1.00 50.51
             7959
                   CG
      MOTA
                                                        19.214
                                                                1.00 52.07
                   CD1 TYR B 123
                                       24.905
                                               66.616
      MOTA
             7960
                                                        20.268
                                                                1.00 56.08
                                       25.759
                                               66.249
                   CE1
                       TYR B 123
             7962
      MOTA
                                                        20.679 1.00 57.64
                       TYR B 123
                                       26.759
                                               67.115
                   CZ
      MOTA
             7964
                                                        21.710 1.00 62.04
                       TYR B 123
                                       27.589
                                               66.754
             7965
                   OH
60
      MOTA
                                                       20.054
                                                               1.00 58.63
                                       26.917
                                               68.341
             7967
                   CE2 TYR B 123
      MOTA
```

| 5 | ATOM | 7969 | CD2 | TYR | B 123 | 26.051 | 68.692 | 19.001 | 1.00 56.37 | | С |
|------|--------------|--------------|----------|-------|----------------|------------------|------------------|----------------|------------|---|------------|
| Ľ. | MOTA | 7971 | С | TYR | в 123 | 21.979 | 69.223 | 16.661 | 1.00 43.80 | | . C |
| | MOTA | 7972 | 0 | TYR | B 123 | 20.957 | 68.637 | 16.350 | 1.00 50.79 | | 0 |
| | MOTA | 7973 | N | | B 124 | 22.477 | 70.250 | 15.982 | 1.00 43.43 | | N |
| | MOTA | 7975 | CA. | | B 124 | 21.793 | 70.841 | 14.838 | 1.00 43.69 | | С |
| 10 | MOTA | 7977 | CB | | B 124 | 22.566 | 72.036 | 14.319 | 1.00 46.07 | | ,C |
| • | MOTA | 7981 | С | | B 124 | 21.612 | 69.869 | 13.717 | 1.00 42.56 | | С |
| | ATOM | 7982 | 0 | ALA | B 124 | 20.594 | 69.882 | 13.067 | 1.00 42.47 | | 0 |
| | ATOM | 7983 | N | GLU | B 125 | 22.582 | 69.006 | 13.476 | 1.00 44.82 | | N |
| | ATOM | 7985 | CA | | В 125 | 22.469 | 68.163 | 12.296 | 1.00 47.99 | , | С |
| 15 | MOTA | 7987 | CB | | B 125 | 23.515 | 67.059 | 12.235 | 1.00 49.37 | | C |
| | MOTA | 7990 | . CG | | B 125 | 22.957 | 65.812 | 11.577 | 1.00 57.34 | | С |
| | ATOM | 7993 | CD | | B 125 | 23.551 | 65.493 | 10.224 | 1.00 64.77 | | С |
| | MOTA | 7994 | | | B 125 | 24.491 | 64.674 | 10.186 | 1.00 71.72 | , | 0 |
| | ATOM | 7995 | | | В 125 | 23.068 | 66.040 | 9.201 | 1.00 74.39 | | 0 |
| 20 | ATOM | 7996 | С | | B 125 | 21.107 | 67.553 | 12.132 | 1.00 44.92 | • | С |
| | MOTA | 7997 | 0 | | B 125 | 20.708 | 67.270 | 11.008 | 1.00 47.91 | | 0 |
| | ATOM | 7998 | N | | B 126 | 20.381 | 67.329 | 13.219 | 1.00 43.01 | | N |
| | ATOM | 8000 | CA | | B 126 | 19.116 | 66.641 | 13.067 | 1.00 40.58 | | С |
| | ATOM | 8002 | CB | | B 126 | 19.078 | 65.412 | 13.969 | 1.00 39.84 | | С |
| 25 | ATOM | 8004 | | | B 126 | 18.870 | 65.776 | 15.413 | 1.00 43.52 | | C |
| | ATOM | 8007 | | | B 126 | 18.662 | 64.549 | 16.288 | 1.00 44.92 | | C |
| • | ATOM | 8011 | | | B 126 | 20.372 | 64.751 | 13.908 | 1.00 40.38 | | С |
| | ATOM | 8015 | С | | B 126 | 17.962 | 67.565 | 13.315 | 1.00 42.42 | | С |
| | ATOM | 8016 | 0 | | B 126 | 16.823 | 67.138 | 13.565 | 1.00 40.90 | | 0 |
| 30 | ATOM | 8017 | N | | В 127 | 18.250 | 68.853 | 13.236 | 1.00 42.86 | | N |
| | MOTA | 8019 | CA | | В 127 | 17.202 | 69.836 | 13.404 | 1.00 42.99 | | С |
| • | ATOM | 8021 | CB | | B 127 | 17.753 | 71.130 | 13.922 | 1.00 44.98 | • | С |
| | ATOM | 8025 | C | | B 127 | 16.525 | 70.059 | 12.091 | 1.00 41.47 | | С |
| 25 | ATOM | 8026 | 0 . | | B 127 | 17.105 | 69.882 | 11.050 | 1.00 39.97 | | 0 |
| 35 | ATOM | 8027 | N | | B 128 | 15.272 | 70.444 | 12.165 | 1.00 44.79 | | N |
| | ATOM | 8029 | CA | | B 128 | 14.517 | 70.755 | 10.990 | 1.00 43.13 | | C |
| | ATOM | 8031 | CB | | 3 128 | 13.282 | 69.894 | 10.960 | 1.00 42.01 | | С |
| | MOTA | 8034 | CG | | 3 128 | 13.574 | 68.400 | 11.101 | 1.00 49.12 | | C |
| 40 | ATOM ATOM | 8037 | CD | | 3 128 | 13.536 | 67.609 | 9.795 | 1.00 52.69 | | C |
| 70 | ATOM | 8040 8042 | NE CZ | | 3 128 3 128 | 13.330 | 66.174 | 10.019 | 1.00 58.75 | | N |
| | ATOM | 8043 | | | 3 128 | 12.511 11.809 | 65.403 | 9.306 | 1.00 61.67 | | C |
| | ATOM | 8046 | | | 3 128 | 12.396 | 65.915 64.110 | 8.308 | 1.00 58.06 | | N |
| | ATOM | 8049 | C | | 3 128 | 14.154 | | 9.592 | 1.00 62.03 | | N |
| 45 | ATOM | 8050 | 0. | | 3 128 | 14.131 | 72.208 72.729 | 11.134 | 1.00 41.86 | | C |
| | ATOM | 8051 | N. | | 3 129 | 13.883 | 72.729 | 12.258 | 1.00 39.07 | | 0 |
| | ATOM | 8052 | | PRO I | | 13.958 | 72.233 | 10.013 | 1.00 42.22 | | N |
| | ATOM | 8054 | | | 3 129 | 13.390 | 73.274 | 8.694 | 1.00 43.56 | | C |
| • | ATOM | 8057 | CG | | 3 129 | 12.704 | 74.249 | 7.755 | 1.00 45.93 | | C |
| 50 - | ATOM | . 8060 | CD | | 3.129 | 13.465 | 74.249 | 8.633 9.924 | 1.00 47.55 | | C |
| 50 | ATOM | 8063 | C | | 3 129 | 15.348 | | | 1.00 43.06 | | . C |
| | ATOM | 8064 | Ö | | 3 129 | 15.524 | 71.893 71.066 | 8.290 7.396 | 1.00 45.94 | | C |
| | ATOM | 8065 | N | | 3 130 | 16.340 | 72.488 | | 1.00 49.70 | | 0 |
| | ATOM | 8067 | CA | | 3 130 | 17.715 | 72.466 | 8,929 | 1.00 51.65 | | N |
| 55 | ATOM | 8069 | СВ | | 3 130 | 18.119 | 72.654 | 8.642 | 1.00 53.34 | | C |
| 55 | ATOM | 8072 | CG | | 3 130 | 18.180 | | 7.330 | 1.00 55.91 | | C, |
| | ATOM | 8073 | | ASP I | | 17.510 | 74.138 74.791 | 7.387 | 1.00 61.07 | | C |
| | ATOM | 8074 | | | 3 130 | 18.856 | 74.731 | 6.545 8.265 | 1.00 72.80 | | 0 |
| | ATOM | 8075 | C | | 3 130 | 18.748 | 72.613 | | 1.00 52.07 | | 0 |
| 60 | ATOM | 8076 | | | 3 130 | 18.515 | 73.579 | 9.600 | 1.00 55.45 | | C . |
| | ATOM | 8077 | N . | | 3 131 | 19.918 | 71.989 | 10.342 | 1.00 58.60 | | 0 |
| | WIOU | | 7.4 | nor I | 121 | 19.910 | 11.989 | 9.529 | 1.00 53.37 | | N |

| | | | | | | | | | | | | | _ |
|-------|--------|----------------|-----|----------|--------------|--------|--------|--------|------|---------|---|---|----|
| 5 | ATOM | 8079 | CA | ASP B 13 | 31 | 21.056 | 72.356 | 10.347 | | 52.86 | | | C |
| • | ATOM | | | ASP B 13 | | 22.321 | 71.615 | 9.849 | 1.00 | 56.83 | | , | С |
| | ATOM | | | ASP B 13 | | 22.898 | 72.170 | 8.499 | 1.00 | 67.88 | | | С |
| | ATOM | | | ASP B 1 | | 22.369 | 73.164 | 7.913 | 1.00 | 71.66 | | | 0 |
| | | | | ASP B 13 | | 23.911 | 71.651 | 7.950 | 1.00 | 67.67 | | | Ó |
| • | ATOM | | | ASP B 13 | | 21.294 | 73.855 | 10.486 | | 47.33 | | | С |
| 10 | ATOM | 8087 | | | | | 74.261 | 11.276 | | 55.44 | | | 0 |
| | MOTA | • | | ASP B 1 | | 22.103 | • | | | 49.22 | | | N |
| | ATOM | 8089 | N | SER B 1 | | 20.599 | 74.692 | 9.743 | | | | | Ċ |
| | MOTA | 8091 | CA | SER B 1 | 32 | 20.799 | 76.144 | 9.863 | | 51.59 | | | C |
| | MOTA | 8093 | CB | SER B 1 | 32 | 20.431 | 76.880 | 8.576 | | 56.09 | | | |
| 15 | MOTA | 8096 | OG | SER B 1 | 32 | 19.064 | 77.316 | 8.672 | | 56.61 | | | 0 |
| 10 | ATOM | 8098 | C · | SER B 1 | 32 . | 19.910 | 76.773 | 10.877 | | 48.16 | | | С |
| | ATOM | 8099 | 0 | SER B 1 | 32 | 19.967 | 77.966 | 11.030 | | 48.29 | | | 0 |
| | MOTA | 8100 | N | LEU B 1 | | 19.044 | 75.996 | 11.514 | 1.00 | 51.70 | | | И |
| • | | 8102 | CA | LEU B 1 | | 18.210 | 76.511 | 12.594 | 1.00 | 48.34 | | | С |
| 00 | ATOM | | | LEU B 1 | | 16.784 | 75.967 | 12.530 | | 50.22 | | | С |
| 20 | MOTA | 8104 | CB | | | 15.867 | 76.770 | 13.479 | | 50.22 | | | С |
| | MOTA | 8107 | CG | LEU B 1 | | | 77.914 | 12.692 | | 51.60 | | | С |
| | MOTA | 8109 | | LEU B 1 | | 15.291 | | | | 46.25 | | | C |
| | ATOM | 8113 | | LEU B 1 | | 14.749 | 75.979 | 14.133 | | 48.97 | | | C |
| - | ATOM | 8117 | C | LEU B 1 | | 18.841 | 76.165 | 13.947 | | | | | 0 |
| 25 | MOTA | 8118 | 0 | LEU B 1 | .33 | 18.549 | 75.164 | 14.561 | | 55.14 | | | |
| | MOTA | 8119 | Ν . | GLU B 1 | 34 | 19.728 | 77.021 | 14.398 | | 51.87 | | | N |
| | ATOM | 8121 | CA | GLU B 1 | | 20.411 | 76,871 | 15.673 | | 49.82 | | | С |
| | ATOM | 8123 | СВ | GLU B 1 | | 21.132 | 78.206 | 15.930 | 1.00 | 52.58 | | | С |
| | ATOM | 8126 | CG | GLU B 1 | | 21.942 | 78.394 | 17.194 | 1.00 | 57.11 | | | C |
| 20 | | | CD | GLU B 1 | | 22.920 | 79.568 | 17.051 | 1.00 | 62.70 | | | С |
| 30 | ATOM . | 8129 | | GLU B 1 | | 23.903 | 79.441 | 16.281 | | 65.85 | | | 0 |
| | ATOM | 8130 | | | | 22.717 | | | | 63.04 | | | 0 |
| • | MOTA | 8131 | | GLU B 1 | | | 76.499 | 16.822 | | 46.15 | | | С |
| | MOTA | 8132 | C | GLU B 1 | | 19.462 | | | | 40.78 | | | o |
| | MOTA | 8133 | 0 ' | GLU B 1 | | 18.509 | 77.230 | 17.070 | | 39.43 | | | N |
| 35 | MOTA | 8134 | Ņ | PRO B 1 | | 19.735 | 75.368 | 17.494 | | | | | C |
| | MOTA | 8135 | CA | PRO B 1 | | 19.040 | | 18.710 | | 40.62 | | | c |
| | ATOM | 8137 | CB | PRO B 1 | 135 | 19.597 | 73.515 | 18.944 | | 39.60 | | | |
| | MOTA | 8140 | CG | PRO B 1 | L 3 5 | 20.409 | | 17.783 | | 40.53 | | | C |
| | ATOM | 8143 | CD | PRO B 1 | L35 | 20.750 | 74.409 | 17.082 | | 41.45 | | | С |
| 40 | ATOM | 8146 | С | PRO B 1 | L35 | 19.301 | 75.722 | 19.982 | | 39.91 | | | С |
| -10 | ATOM | 8147 | Ō | PRO B 1 | | 20.327 | | 20.169 | 1.00 | 42.53 | | | 0 |
| | ATOM | 8148 | N | PHE B | | 18.361 | | 20.906 | 1.00 | 44.02 | • | | N |
| | | 8150 | CA | PHE B 1 | | 18.396 | | 22.119 | 1.00 | 44.27 | | | C |
| | ATOM | | CB | PHE B 3 | | 17.279 | | | 1.00 | 41.68 | | | C. |
| 45 | MOTA | 8152 | | PHE B | | 17.309 | | | | 39.04 | | | С |
| 45 | MOTA | 8155 | CG | | | | | | | 40.01 | | | C |
| | MOTA | 8156 | | PHE B | | 16.639 | | | - | 43.44 | | | C |
| | | · 81 58 | • | PHE B | | 16.683 | | | | 46.05 | | | č |
| | MOTA | 8160 | | PHE B | | 17.417 | | | | | | | Ċ. |
| | MOTA | · 8162 | CE2 | PHE B | 136 | 18.113 | | | | 43.71 | | | |
| 50 | MOTA | 8164 | CD2 | PHE B | 136 | 18.056 | 76.545 | | | 44.61 | | | C |
| • | ATOM | 8166 | С | PHE B | | 19.672 | 76.460 | 22.926 | 1.00 | 42.84 | | | C |
| | ATOM | 8167 | 0 | PHE B | | 20.091 | | 23.427 | 1.00 | 44.70 | | | 0 |
| | | 8168 | N | PHE B | | 20.282 | | 23.088 | 1.00 | 44.28 | | | N |
| | ATOM | | CA | PHE B | | 21.496 | | | | 45.73 | | | C |
| ہز ہے | ATOM | 8170 | | | | | | | | 46.94 | | | C |
| 55 | ATOM | 8172 | CB | PHE B | | 21.819 | | | | 45.95 | | | Ċ |
| | ATOM | 8175 | CG | PHE B | | 22.697 | | | | | | | c |
| | ATOM | 8176 | | L PHE B | | 22.194 | | | | 47.44 | | | C |
| | MOTA | 8178 | | L PHE B | | 23.019 | | | | 47.99 | | | |
| | ATOM | 8180 | CZ | PHE B | | 24.338 | | | | 36.10 | | | C |
| 60 | ATOM | 8182 | CE | 2 PHE B | 137 | 24.842 | | | | 37.75 | | | C |
| 30 | ATOM | 8184 | | 2 PHE B | | 24.04 | | 25.394 | 1.00 | 3 45.95 | | • | С |
| | AIOM | | | | | • - | | | | | | | |

| | | | | | | | | | | 1 00 | 43.32 | | | С |
|----|-------|------|------|-------|-------|---|--------|--------|----------------|------|---------|---|---|----|
| 5 | MOTA | 8186 | С | PHE E | | | 22.696 | 75.938 | 23.216 | | | | | |
| | MOTA | 8187 | 0 | PHE E | 3 137 | • | 23.468 | 76.599 | 23.887 | | 42.97 | : | | 0 |
| | ATOM | 8188 | N | ASP E | | | 22.843 | 75.783 | 21.895 | 1.00 | 44.54 | | | N |
| | | | | ASP E | | | 23.891 | 76.481 | 21.156 | 1.00 | 37.01 | | | С |
| | MOTA | 8190 | CA | | | | | 76.253 | 19.706 | | 35.76 | | | Ç |
| | MOTA | 8192 | CB | ASP I | | | 23.736 | | | | 41.96 | | | Ċ |
| 10 | MOTA | 8195 | CG | ASP F | | | 24.247 | 74.993 | 19.282 | | | | | ŏ |
| | MOTA | 8196 | OD1 | ASP I | 3 138 | | 25.187 | 75.024 | 18.467 | | 61.10 | | | |
| | ATOM | 8197 | | ASP I | | | 23.796 | 73.908 | 19.672 | | 56.89 | | | 0 |
| | ATOM | 8198 | C | | 3 138 | | 23.788 | 77.995 | 21.316 | 1.00 | 43.61 | | | С |
| | | | | | 3 138 | | 24.743 | 78.650 | 21.697 | 1.00 | 47.84 | | | 0 |
| | MOTA | 8199 | 0 | | | | | 78.554 | 20.991 | | 46.65 | | | N |
| 15 | MOTA | 8200 | N | | 3 139 | | 22.626 | | | | 48.26 | | | C |
| | ATOM | 8202 | CA | | 3 139 | • | 22.433 | 79.979 | 21.115 | | | | | č |
| | MOTA | 8204 | CB | SER I | в 139 | | 21.004 | 80.383 | 20.742 | | 51.54 | | | |
| | ATOM | 8207 | OG | SER I | в 139 | | 20.647 | 79.872 | 19.469 | | 51.53 | | | 0 |
| • | ATOM | 8209 | С | | в 139 | | 22.691 | 80.372 | 22.526 | 1.00 | 48.43 | | | С |
| 20 | | | | | В 139 | | 23.245 | 81.423 | 22.774 | 1.00 | 49.51 | | | 0 |
| 20 | MOTA | 8210 | 0 | | | | 22.286 | 79.537 | 23.470 | | 52.62 | | | N |
| | MOTA | 8211 | N | | В 140 | | | | 24.874 | | 56.48 | | | С |
| | MOTA | 8213 | CA | | B-140 | • | 22.480 | 79.895 | | | 56.51 | | | ·C |
| | MOTA | 8215 | CB | LEU : | В 140 | | 21.930 | 78.831 | 25.813 | | | | | |
| | MOTA | 8218 | CG | LEU : | B 140 | | 22.375 | 79.194 | 27.234 | | 54.72 | | | С |
| 25 | ATOM | 8220 | | LEU | В 140 | | 21.590 | 80.369 | 27.719 | 1.00 | 55.46 | | | С |
| 23 | | 8224 | | | B 140 | | 22.222 | 78.095 | 28.210 | 1.00 | 57.48 | | • | С |
| | ATOM | | | | | | 23.955 | 80.086 | 25.211 | | 57.93 | | | С |
| | MOTA | 8228 | С | | B 140 | | | | 25.897 | | 59.89 | | | .0 |
| | ATOM | 8229 | 0 | | | | 24.333 | 81.037 | | | | | | N |
| | MOTA | 8230 | N | VAL | B 141 | | 24.793 | 79.168 | 24.751 | | 55.68 | | | |
| 30 | ATOM | 8232 | CA | VAL | B 141 | | 26.196 | 79.300 | 25.021 | | 54.58 | | | С |
| - | ATOM | 8234 | CB | VAL | B 141 | | 26.883 | 78.025 | 24.692 | | 58.69 | | | С |
| | ATOM | 8236 | | | В 141 | | 28.370 | 78.251 | 24.440 | 1.00 | 58.03 | | | С |
| | | | | | B 141 | | 26.664 | 77.039 | | 1.00 | 61.23 | | | C. |
| | MOTA | 8240 | | | | | 26.822 | 80.452 | 24.243 | | 57.01 | | | С |
| | MOTA | 8244 | С | | B 141 | | | | 24.817 | | 58.33 | | | 0 |
| 35 | MOTA | 8245 | 0 | | B 141 | | 27.587 | 81.229 | | | 54.66 | | | N |
| | ATOM | 8246 | N | LYS | B 142 | | 26.517 | 80.585 | 22.948 | | | | • | C |
| | ATOM | 8248 | CA | LYS | B 142 | • | 27.109 | 81.677 | 22.188 | | 51.01 | | | |
| | MOTA | 8250 | CB | LYS | B 142 | | 26.710 | 81.694 | 20.673 | | 47.84 | | | С |
| | ATOM | 8253 | CG | | B 142 | | 27.455 | 80.681 | 19.723 | 1.00 | 48.68 | | | С |
| 40 | | 8256 | CD | | B 142 | | 26.743 | 80.426 | 18.329 | 1.00 | 54.09 | | | С |
| 40 | MOTA | | | | B 142 | | 27.275 | 79.184 | 17.438 | 1.00 | 59.89 | | | C |
| | MOTA | 8259 | CE | | | | | 77.779 | 17.577 | | 63.41 | | | N |
| | MOTA | 8262 | NZ | | B 142 | | 26.633 | | | | | • | | C |
| | MOTA | 8266 | С | | B 142 | | 26.755 | 82.966 | 22.952 | | 49.96 | | | ő |
| | ATOM | 8267 | 0 | LYS | B 142 | | 27.616 | 83.791 | 23.156 | | 61.21 | | | |
| 45 | ATOM | 8268 | N | GLN | B 143 | | 25.521 | 83.104 | 23.424 | | 50.78 | | | N |
| | MOTA | 8270 | CA | | в 143 | | 24.976 | 84.369 | 24.029 | 1.00 | 49.37 | | | С |
| | | 8272 | | | B 143 | | 23.414 | 84.421 | 23.829 | 1.00 | 45.79 | | | С |
| | MOTA | | | | | | 22.945 | | - - | | 0 47.31 | | | С |
| | MOTA | 8275 | CG | | B 143 | | | | | | 0 47.17 | | | С |
| | MOTA. | 8278 | | | B 143 | | 21.414 | | | | | | | ŏ |
| 50 | MOTA | 8279 | OE I | GLN | B 143 | | 20.610 | | 22.936 | | 0 50.01 | | | |
| | MOTA | 8280 | | GLN | B 143 | | 21.028 | 84.304 | 20.937 | 1.0 | 0 42.57 | | | N |
| | ATOM | 8283 | | | в 143 | | 25.276 | 84.719 | 25.510 | 1.0 | 0 49.46 | | • | С |
| • | | | | | B 143 | | 24.919 | | | | 0 53.59 | | | 0 |
| | ATOM | 8284 | 0. | | | | | | | | 0 54.02 | | | N |
| | ATOM | 8285 | | | B 144 | | 25.887 | | | | | | | C |
| 55 | MOTA | 8287 | CA | THR | B 144 | • | 26.271 | 84.125 | | | 0 56.45 | | | |
| | ATOM | | CB | THR | B 144 | | 25.218 | | | | 0 58.45 | | | C |
| | ATOM | | | | B 144 | | 25.574 | 82.273 | 29.043 | 1.0 | 0 57.95 | | | 0 |
| | | | | | В 144 | | 23.847 | | | 1.0 | 0 57.06 | | | C |
| | MOTA | | | | В 144 | | 27.659 | | | | 0 62.87 | | | С |
| | ATOM | | | | | | | | | | 0 65.39 | | | 0 |
| 60 | MOTA | | | THR | B 144 | | 28.354 | | | | 0 65.98 | | | N |
| | MOTA | 8299 | N | HIS | В 145 |) | 28.091 | 83.348 | 29.179 | 1.0 | 05.30 | | | ., |
| | | | | | | | | | | | | | | |

| 5 | ATOM | 8301 | CA | HIS | B 145 | | 29.387 | 82.706 | | | 74.26 | | C |
|-----------|------|------|-----|-------|---------------|---|--------|--------|--------|-------|-------|---|-------|
| _ | ATOM | 8303 | СВ | HIS I | B 145 | - | 30.175 | 83.559 | 30.474 | | | - | С |
| | MOTA | 8306 | CG | HIS ! | B 1 45 | | 30.447 | 84.988 | 30.036 | | 86.80 | | С |
| | MOTA | 8307 | ND1 | HIS 1 | B 145 | | 29.853 | 86.089 | 30.629 | | 87.60 | | N |
| | MOTA | 8309 | CE1 | HIS | B 145 | | 30.285 | 87.194 | 30.045 | | 87.90 | | C |
| 10 | MOTA | 8311 | NE2 | HIS ! | в 145 | | 31.142 | 86.856 | 29.099 | | 89.90 | | N |
| | ATOM | 8313 | CD2 | HIS I | B 145 | | 31.263 | 85.486 | 29.073 | | 88.35 | | С |
| | ATOM | 8315 | С | HIS | B 145 | | 29.243 | 81.228 | 29.905 | | 71.71 | | С |
| | ATOM | 8316 | 0 | HIS : | В 145 | | 30.212 | 80.600 | 30.363 | | 71.89 | | .0 |
| | ATOM | 8317 | N | VAL | B 146 | | 28.031 | 80.682 | 29.754 | | 66.58 | | N |
| 15 | ATOM | 8319 | CA | VAL | B 146 | | 27.678 | 79.350 | 30.230 | | 58.14 | | С |
| 10 | ATOM | 8321 | | | B 146 | | 26.233 | 79.064 | 29.905 | | 59.42 | | C |
| | ATOM | 8323 | | | B 146 | | 25.936 | 77.582 | 29.997 | | 62.47 | | С |
| | ATOM | 8327 | | | B 146 | | 25.357 | 79.864 | 30.838 | | 57.89 | | C |
| | ATOM | 8331 | C | | В 146 | | 28.537 | 78.328 | 29.562 | | 54.48 | | С |
| 20 | ATOM | 8332 | | | B 146 | | 28.531 | 78.205 | 28.337 | | 59.51 | | 0 |
| 2.0 | ATOM | 8333 | N | | B 147 | | 29.288 | 77.580 | 30.359 | | 51.96 | | N |
| | ATOM | 8334 | CA | | в 147 | | 30.138 | 76.562 | 29.777 | | 49.03 | | C |
| | MOTA | 8336 | CB | | B 147 | | 30.757 | 75.883 | 30.985 | 1.00 | 46.35 | | C |
| | ATOM | 8339 | CG | | в 147 | | 30.725 | 76.871 | 32.008 | | 44.84 | | С |
| 25 | ATOM | 8342 | CD | | B 147 | | 29.404 | 77.576 | 31.827 | | 51.63 | | С |
| 25 | ATOM | 8345 | c | | в 147 | | 29.250 | 75.614 | 29.019 | 1.00 | 51.04 | | С |
| | ATOM | 8346 | ō | | B 147 | | 28.120 | 75.312 | 29.390 | 1.00 | 56.78 | | 0 |
| | ATOM | 8347 | N | | B 148 | | 29.782 | 75.143 | 27.923 | 1.00 | 45.46 | | N |
| | ATOM | 8349 | CA | | B 148 | - | 29.006 | 74.373 | 27.015 | 1.00 | 41.55 | • | С |
| 30 | ATOM | 8351 | CB | | B 148 | | 29.683 | 74.441 | 25.664 | 1.00 | 43.45 | | С |
| 50 | ATOM | 8354 | CG | | B 148 | | 28.986 | 73.682 | 24.627 | 1.00 | 41,45 | | С |
| | ATOM | 8355 | | | B 148 | | 27.770 | 73.450 | 24.682 | 1.00 | 44.14 | | 0 |
| | ATOM | 8356 | | | в 148 | | 29.744 | 73.296 | 23.627 | 1.00 | 37.99 | | N |
| | ATOM | 8359 | С | | B 148 | | 28.991 | 72.993 | 27.538 | | 43.05 | | С |
| 35 | ATOM | 8360 | o · | | B 148 | | 29.608 | 72.076 | 26.973 | 1.00 | 40.55 | | 0 |
| 33 | ATOM | 8361 | N | | B 149 | | 28.283 | 72.847 | 28.648 | 1.00 | 42.80 | | N |
| | ATOM | 8363 | CA | | В 149 | | 28.132 | 71.521 | 29.273 | 1.00 | 41.70 | | С |
| | ATOM | 8365 | CB. | | B 149 | | 29.275 | 71.263 | 30.278 | 1.00 | 39.84 | | С |
| | ATOM | 8368 | CG | | B 149 | | 29.338 | 69.945 | 31.031 | 1.00 | 41.12 | | С |
| 40 | ATOM | 8370 | | | B 149 | | 30.675 | 69.702 | | 1.00 | 39.27 | | С |
| | ATOM | 8374 | | | В 149 | | 28.368 | 69.844 | 32.185 | 1.00 | 43.77 | | C |
| | ATOM | 8378 | C | | в 149 | | 26.812 | 71.556 | 30.000 | 1.00 | 42.18 | | С |
| • | ATOM | 8379 | 0 | | В 149 | | 26.391 | 72.623 | 30.409 | 1.00 | 48.04 | | 0 |
| | ATOM | 8380 | N | PHE | B 150 | | 26.128 | 70.428 | 30.161 | 1.00 | 37.65 | | N |
| 45 | ATOM | 8382 | CA | | в 150 | | 24.982 | 70.422 | 31.068 | | 39.61 | | С |
| | MOTA | 8384 | CB | PHE | B 150 | | 23.718 | 70.954 | 30.396 | 1,.00 | 40.04 | | С |
| | ATOM | 8387 | CG | | в 150 | | 23.235 | 70.093 | 29.272 | 1.00 | 41.92 | | С |
| | ATOM | 8388 | CD1 | | B 150 | | 23.411 | 70.479 | 27.963 | 1.00 | 40.21 | • | С |
| | ATOM | 8390 | CE1 | | B 150 | | 22.976 | 69.678 | 26.938 | 1.00 | 37.50 | | С |
| 50 | ATOM | 8392 | CZ | | в 150 | | 22.352 | 68.486 | 27.193 | 1.00 | 45.37 | | С |
| 50 | MOTA | 8394 | | | B 150 | | 22.165 | 68.070 | 28.490 | 1.00 | 40.66 | | . C |
| | ATOM | 8396 | | | B 150 | | 22.608 | | 29.526 | 1.00 | 38.93 | | С |
| | ATOM | 8398 | C | | В 150 | | 24.829 | | 31.584 | 1.00 | 42.19 | | С |
| | ATOM | 8399 | ŏ | | B 150 | | 25.195 | | 30.883 | 1.00 | 41.76 | | 0 |
| 55 | ATOM | 8400 | N | | B 151 | | 24.321 | 68.798 | 32.803 | 1.00 | 37.28 | | N |
| , ,,, | MOTA | 8402 | CA | | B 151 | • | 24.135 | | 33.313 | | 42.07 | | С |
| | ATOM | 8404 | CB | | B 151 | | 25.051 | | | | 38.99 | | С |
| | ATOM | 8407 | OG | | B 151 | | 25.053 | | 35.324 | | 34.21 | | 0 |
| | | 8409 | C | | B 151 | | 22.671 | | | | 43.06 | | С |
| 60 | MOTA | 8410 | ŏ | | B 151 | | 21.970 | | | | 45.97 | | 0 |
| UU | MOTA | 8411 | N | | B 152 | | 22.207 | | | | 40.15 | | N |
| | MOTA | CATT | 7.4 | TIE (| בעב ע | | | | | | | | |

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1.00 40.34
                                                        34.122
                                       20.832 65.747
                       LEU B 152
            8413
                  CA
     ATOM
                                                                 1.00 42.16
                                                        32.938
                                       19.975 .65.313
                  CB
                       LEU B 152
            8415
     MOTA
                                                        31.756
                                                                 1.00 38.97
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                                               66.186
                       LEU B 152
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                                                                                       C
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                                                                 1.00 40.87
                                       18.685
                                               65.352
                  CD1 LEU B 152
            8420
     MOTA
                                                                 1.00 38.15
                                                                                       С
                                                        32.159
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                                               67.410
                  CD2 LEU B 152
     ATOM
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                                                                 1.00 39.44
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                       LEU B 152
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                                                64.628
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                       LEU B 152
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                       GLN B 153
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                                                64.855
                  N
     ATOM
            8430
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            8432
                  CA
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                                                64.202
                       GLN B 153
            8434
                  CB
     MOTA
                                                                                       С
                                                                 1.00 43.66
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                                                63.157
                                                        39.636
                       GLN B 153
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                   CG
15
     MOTA
                                                                                       C
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                                      19.775
                                                63.765
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     ATOM
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                   CD
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                                                                                       0
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                                     20.437
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                                                        37.191
                                                                 1.00 44.67
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            8445
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                                                                                        0
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                   0
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                                                                                        N
                                                                 1.00 45.13
                                                        36.510
                                       17.803
                                                62.538
                       LEU B 154
            8447
                   N
     ATOM
                                                                                        C
                                                62.281
                                                        36.551
                                                                 1.00 40.93
                                       16.364
                       LEU B 154
            8449
                   CA
     ATOM
                                                                                        C
                                                        35.270
                                                                 1.00 37.85
                                       15.907
                                                61.599
                       LEU B 154
            8451
                   CB
     MOTA
                                                                                        C
                                       16.262
                                                62.308
                                                        33.959
                                                                 1.00 35.17
                       LEU B 154
             8454
                   CG
     MOTA
                                                                 1.00 32.97
                                                                                        C
                                                        32.748
                   CD1 LEU B 154
                                       15.572
                                                61.588
25
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                                                                                        C
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                       LEU B 154
     MOTA
                                                                                        С
                                                                 1.00 49.47
                                                         37.707
                                       16.081
                       LEU B 154
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             8464
                   С
     MOTA
                                                                                        0
                                                         37.889
                                                                 1.00 54.75
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                                                60.349
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     ATOM
                                                                                        N
                                                         38.490
                                                                 1.00 52.56
                                       15.044
                                                61.606
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                       CYS B 155
     ATOM
                   N
                                                                                        С
                                                60.747
                                                         39.622
                                                                 1.00 56.72
                                       14.695
                       CYS B 155
30
     ATOM
             8468
                   CA
                                                                 1.00 57.35
                       CYS B 155
                                       14.662
                                                61.539
                                                         40.934
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                   \mathbf{CB} \cdot
     MOTA
                                                                 1.00 67.57
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                       CYS B 155
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                                                62.120
             8473
     MOTA
                                                                                        С
                                                         39.473
                                                                 1.00 58.59
                                       13.353
                                                60.028
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                       CYS B 155
                   С
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                                                                                        0
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                                     12.271
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                        CYS B 155
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                                                                                        N
                                                         39.352
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                                                58.707
                        GLY B 156
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35
     MOTA
                                                                  1.00 58.92
                                                                                        C
                                                         39.443
                       GLY B 156
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     ATOM
                                                                  1.00 58.63
                                                                                        C
                                       11.860
                                                57.937
                                                         40.923
                        GLY B 156
                   С
             8481
     MOTA
                                                         41.741
                                                                                        0
                                                                  1.00 56.21
                   0
                        GLY B 156
                                        12.749
                                                58.009
             8482
     ATOM
                                                                  1.00 62.17
                                                                                        N
                                                         41.288
                                        10.591
                                                57.864
     MOTA
             8483
                   N
                        ALA B 157
                                                                                        C
                                                         42.709
                                        10.255
                                                57.778
                                                                  1.00 64.46
                        ALA B 157
             8485
                   CA
40
     MOTA
                                                                                        C
                                                                  1.00 63.92
                                                         43.026
                        ALA B 157
                                        9.080
                                                58.650
             8487
                   CB
     MOTA
                                                         43.211
                                                                  1.00 66.10
                                        10.022
                                                56.338
                        ALA B 157
             8491
                   С
      MOTA
                                                         44.426
                                                                  1.00 64.25
                                        9.966
                                                56.114
                        ALA B 157
                   0
      MOTA
             8492
                                                                                        Ň
                                                         42.284
                                                                  1.00 66.93
                                                55.383
                        GLY B 158
                                        9.883
             8493
                   N
      MOTA
                                                                  1.00 69.42
                                                                                         С
                                                         42.636
                                                 53.966
             8495
                   CA
                        GLY B 158
                                        9.804
45
     MOTA
                                                                                         С
                                                         43.351
                                                                  1.00 70.66
                                                53.537
                                        8.530
                        GLY B 158
     ATOM
             8498
                   С
                                                                                         0
                        GLY B 158
                                         8.531
                                                 52.749
                                                         44.322
                                                                  1.00 69.74
             8499
                   0
      MOTA
                                                                                         N
                                                                  1.00.70.60
                                                 54.080
                                                         42.826
                        PHE B 159
                                         7.441
             8500
                   N
      MOTA
                                                                                         C
                                         6.078
                                                 53.846
                                                         43.273
                                                                  1.00 71.27
                        PHE B 159
                   CA
      MOTA
             8502
                                                                  1.00 69.71
                                                                                         С
                                                         44.813
                                         5.883
                                                 53.920
                        PHE B 159
50
                   CB
     ATOM
             8504
                                                                                         С
                                                         45.427
                                                                  1.00 64.66
                                                 55.263
                   CG
                        PHE B 159
                                         6.184
             8507
      MOTA
                                                                                         C
                                                                  1.00 61.90
                                                         46.334
                        PHE B 159
                                         7.228
                                                 55.397
             8508
                   CD1
      ATOM
                                                                                         С
                                       ' 7.521
                                                         46.919
                                                                  1.00 65.05
                                                 56.634
      MOTA
             8510
                   CE1
                        PHE B 159
                                                                                         С
                                       6.751
                                                 57.756
                                                         46.599
                                                                  1.00 68.53
                    CZ
                        PHE B 159
      MOTA
             8512
                                                                                         С
                                                         45.694
                                                                  1.00 67.06
                                         5.690
                                                 57.631
                        PHE B 159
55
             8514
                    CE2
      ATOM
                                                                                         C
                                                 56.383
                                                         45.115
                                                                  1.00 66.54
                                         5.414
                    CD2 PHE B 159
             8516
      MOTA
                                                                  1.00 71.04
                                                          42.502
                        PHE B 159
                                         5.311
                                                 54.914
      ATOM
             8518
                    С
                                                 55.974
                                                          42.212
                                                                  1.00 68.13
                        PHE B 159
                                         5.851
             8519
                    0
      MOTA
                                                                  1.00 71.26
                                                          42.157
                                         4.064
                                                 54.657
              8520
                    N
                        PRO B 160
      ATOM
                                                          41.283
                                                                  1.00 72.10
                                                 55.586
                                         3.361
 60
              8521
                    CA
                        PRO B 160
      ATOM
                                                 54.812
                                                          40.899
                                                                  1.00 72.89
                                         2.102
                        PRO B 160
      MOTA
              8523
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| - | 2 0014 | 0506 | CC | PRO B | 160 | | 2.325 | 53.429 | 41.341 | 1.00 71.93 | • | C |
|-----|--------|------|-----|-------|----------------|---|-----------------|--------|--------|------------|----|-----|
| . 5 | MOTA | 8526 | | PRO B | | • | 3.218 | 53.519 | 42.533 | 1.00 69.92 | | .C |
| | ATOM | 8529 | | PRO B | | | 2.959 | 56.894 | 41.919 | 1.00 71.65 | | С |
| | ATOM | 8532 | | PRO B | | | | 57.045 | 43.136 | 1.00 72.02 | | 0 |
| | MOTA | 8533 | | LEU B | | | 2.703 | 57.841 | 41.039 | 1.00 71.52 | ٠. | N |
| 10 | MOTA | 8534 | | LEU B | | | 2.108 | 59.104 | 41.403 | 1.00 75.59 | | С |
| 10 | ATOM | 8536 | | LEU B | | | 3.160 | 60.196 | 41.575 | 1.00 77.46 | | С |
| | ATOM | 8538 | | LEU B | | | 4.493 | 59.938 | 42.269 | 1.00 78.23 | | С |
| | ATOM | 8541 | | LEU B | | | 5.608 | 60.398 | 41.338 | 1.00 78.97 | | С |
| | ATOM | 8543 | | LEU B | | | 4.570 | 60.663 | 43.611 | 1.00 75.00 | | С |
| | ATOM | 8547 | | | | | 1.177 | 59.500 | 40.252 | 1.00 76.43 | | С |
| 15 | ATOM | 8551 | С | LEU B | | | 1.492 | 59.322 | 39.071 | 1.00 79.99 | | 0 |
| | ATOM | 8552 | 0 | LEU B | | | 0.016 | 60.022 | 40.584 | 1.00 75.26 | | N |
| | MOTA | 8553 | N | GLN B | | | | 60.579 | 39.563 | 1.00 75.96 | | С |
| | ATOM | 8555 | CA | GLN B | | | -2.266 | 60.698 | 40.126 | 1.00 75.84 | • | С |
| | MOTA | 8557 | CB | GLN B | | | -2.200 | 61.141 | 41.592 | 1.00 72.01 | | С |
| 20 | MOTA | 8560 | CG | GLN B | | • | -2.514 -1.628 | 62.471 | 41.822 | 1.00 71.95 | | С |
| | MOTA | 8563 | CD | GLN B | | - | -0.588 | 62.767 | 41.223 | 1.00 69.09 | | 0 |
| | ATOM | 8564 | | GLN B | | | -2.203 | 63.281 | 42.696 | 1.00 72.77 | | N |
| | ATOM | 8565 | | GLN B | | | -0.290 | 61.961 | 39.102 | 1.00 77.71 | | · C |
| | MOTA | 8568 | C | GLN B | | : | | 62.153 | 39.019 | 1.00 79.30 | | 0 |
| 25 | MOTA | 8569 | 0 | GLN B | | | 0.933 -1.163 | 62.133 | 38.811 | 1.00 74.89 | | N |
| | MOTA | 8570 | N | GLN B | | | -0.706 | 64.215 | 38.347 | 1.00 76.31 | | С |
| | ATOM | 8572 | CA | GLN B | | | -1.665 | 64.799 | 37.275 | 1.00 74.58 | | C |
| | MOTA | 8574 | CB | GLN B | | | -1.457 | 66.276 | 36.955 | 1.00 75.98 | | C |
| | ATOM | 8577 | CG | GLN B | | | -1.437 | 66.679 | 35.491 | 1.00 78.50 | | С |
| -30 | ATOM | 8580 | CD | GLN B | | | -2.869 | 66.428 | 34.982 | 1.00 73.62 | | . 0 |
| | MOTA | 8581 | | GLN E | | | -0.797 | 67.316 | 34.828 | 1.00 77.14 | | N |
| | ATOM | 8582 | | GLN E | | | -0.797 | 65.139 | 39.566 | 1.00 78.42 | | · C |
| | MOTA | 8585 | C | GLN E | | | 0.544 | 65.807 | 39.667 | 1.00 84.37 | | 0 |
| | MOTA | 8586 | 0 | GLN E | | | -1.452 | 65.154 | 40.501 | 1.00 76.38 | | N |
| 35 | ATOM | 8587 | N | SER E | | | -1.369 | 66.023 | 41.690 | 1.00 73.78 | | С |
| | MOTA | 8589 | CA | SER E | | | -2.442 | 65.635 | 42.714 | 1.00 71.78 | | С |
| | ATOM | 8591 | CB | | 3 164 | | -2.807 | 66.743 | 43.533 | 1.00 71.79 | | 0 |
| | ATOM | 8594 | OG | | 3 164 3 164 | | -0.014 | 65.965 | 42.395 | 1.00 76.38 | | С |
| 40 | ATOM | 8596 | C | | 3 164 | | 0.467 | 66.969 | 42.942 | 1.00 71.19 | | 0 |
| 40 | ATOM | 8597 | 0 | | 3 165 | | 0.590 | 64.778 | 42.378 | 1.00 78.65 | | · N |
| | ATOM | 8598 | N | | B 165 | | 1.805 | 64.521 | 43.125 | 1.00 82.23 | | С |
| | MOTA | 8600 | CA | | B 165 | | 1.948 | 63.017 | 43.344 | 1.00 86.01 | | С |
| • | ATOM | 8602 | CB | | B 165 | | 0.848 | 62.399 | 44.201 | 1.00 88.14 | | . C |
| 46 | MOTA | 8605 | CG | | B 165 | | 1.063 | 60.911 | 44.445 | 1.00 90.26 | | С |
| 45 | ATOM | 8608 | CD | GLU I | | | 2.025 | 60.560 | 45.159 | 1.00 87.30 | | 0 |
| | MOTA | 8609 | | GLU I | | | 0.266 | 60.089 | 43.928 | 1.00 95.66 | | 0 |
| | MOTA | 8610 | | | B 165 | | 3.053 | 65.082 | 42.436 | 1.00 81.15 | | С |
| | MOTA | 8611 | C | | B 165 | | 3.975 | • | 43.096 | 1.00 76.40 | | 0 |
| 50 | ATOM | 8612 | 0 | | | | 3.080 | 64.989 | 41.111 | 1.00 79.40 | | N |
| 50 | ATOM | 8613 | N | | B 166 | | 4.196 | 65.532 | 40.338 | 1.00 77.43 | | C |
| | MOTA | 8615 | CA | | B 166 | | 4.063 | 65.124 | | 1.00 75.19 | | . C |
| | ATOM | 8617 | CB | | B 166 | | 4.836 | | | 1.00 77.04 | | . C |
| | ATOM | 8619 | | VAL | | | 4.538 | | | 1.00 74.6 | | С |
| | ATOM | 8623 | | VAL | | | | | | 1.00 75.4 | | C |
| 55 | MOTA | 8627 | C | | B 166 | | 4.353 | | | 1.00 75.6 | | 0 |
| | ATOM | 8628 | 0 | | B 166 | | 5.468 | | _ | | | N |
| | MOTA | 8629 | N | | B 167 | | 3.259 | | | | | C |
| | MOTA | 8631 | CA | | B 167 | | 3.348 | | | | | Č |
| | ATOM | 8633 | CB | | B 167 | | 1.977 | | | | | č |
| 60 | MOTA | 8636 | | LEU | | | 1.248 | | | | | Č |
| | MOTA | 8638 | CD: | L LEU | R T01 | | -0.170 | 70.303 | JJ.474 | 1.00 77.2 | • | - |

```
1.00 82.87
                                                        38.282
                                        2.047
                                               70.399
            8642
                  CD2 LEU B 167
     ATOM
                                                                1.00 73.27
                                      3.887
                                                        42.302
                                               69.644
            8646
                 C ... LEU B 167
     MOTA
                                                        42.476
                                                                1.00 69.74
                                                                                       0
                                               70.643
                                       4.593
                       LEU B 167
            8647
                  0
     ATOM
                                                                                       N
                                                                1.00 73.73
                                               68.848
                                                        43.288
                                        3.543
                       ALA B 168
            8648
                  N
     ATOM
                                                                                       С
                                                                 1.00 77.27
                                                        44.636
                                        3.962
                                               69.147
                       ALA B 168
                  CA
     ATOM
            8650
                                                                                       С
                                                                 1.00 75.98
                                               68.585
                                                        45.638
                       ALA B 168
                                        2.949
                  CB
10
     ATOM
            8652
                                                                                       С
                                                        44.921
                                                                 1.00 78.89
                                               68.596
                       ALA B 168
                                        5.353
                  C
            8656
     MOTA
                                                                                       0
                                                                 1.00 84.58
                                               69.005
                                                        45.889
                                        5.995
                  0
                       ALA B 168
            8657
     ATOM
                                                                 1.00 76.97
                                                                                       N
                                               67.688
                                                        44.083
                                        5.832
                       SER B 169
            8658
                  N
     MOTA
                                                                 1.00 77.52
                                                                                       С
                                                        44.373
                                                67.029
                                        7.094
                       SER B 169
     ATOM
            8660
                   CA
                                                                                       С
                                                                 1.00 80.08
                                               65.549
                                                        44.637
                       SER B 169
                                        6.858
            8662
                   CB
15
     MOTA
                                                                                       0
                                                                 1.00 83.47
                                                        45.312
                       SER B 169
                                        5.612
                                                65.396
     MOTA
            8665
                   OG
                                                                                       C
                                                                 1.00 75.54
                                                        43.285
                                                67.204
                       SER B 169
                                        8.122
                   С
            8667
     MOTA
                                                                                       0
                                                                 1.00 69.75
                                                         42.162
                                                67.604
                                        7.817
                       SER B 169
            8668
                   0
     MOTA
                                                                 1.00 74.47
                                                                                       N
                                        9.355
                                                66.890
                                                         43.658
                       VAL B 170
            8669
                   N
     MOTA
                                                                                       С
                                                                 1.00 73.73
                                                         42.805
                                                67.097
                                       10.511
                       VAL B 170
            8671
                   CA
20
     MOTA
                                                                                       С
                                                         43.675
                                                                 1.00 72.68
                       VAL B 170
                                       .11.777
                                                67.421
             8673
                   CB
     MOTA
                                                                                       С
                                                                 1.00 74.83
                                                67.140
                                                         42.959
                                       13.078
                   CG1 VAL B 170
            8675
     MOTA
                                                                                       С
                                                                 1.00 72.94
                                                         44.098
                   CG2 VAL B 170
                                       11.755
                                                68.881
             8679
     ATOM
                                     10.654
                                                                                       С
                                                65.893
                                                                 1.00 71.65
                                                         41.861
                       VAL B 170
             8683 - C
     MOTA
                                                                                       0
                                                         42.012
                                                                 1.00 75.35
                                                64.866
                                       9.950
25
             8684
                   0
                       VAL B 170
     ATOM
                                                                 1.00 64.10
                                       11.525
                                                66.035
                                                         40.863
                       GLY B 171
     MOTA
             8685
                   N
                                                                 1.00 57.27
                                                                                        C
                                                         39.890
                                       11.730
                                                64.987
                       GLY B 171
             8687
                   CA
     MOTA
                                                         39.419
                                                                 1.00 52.94
                                                                                        С
                                       13.146
                                                64.918
                       GLY B 171
             8690
                   C
      MOTA
                                                                                        0
                                                                 1.00 50.16
                                                64.116
                                                         38.563
                       GLY B 171
                                       13.434
      MOTA
             .8691
                   0
                                                                                        N
                                                                 1.00 48.11
                                                         39.959
                       GLY B 172
                                       14.024
                                                65.757
30
             8692
                   N
     · ATOM
                                                                                        С
                                                         39.591
                                                                 1.00 48.37
                                                65.704
                                       15.412
             8694
                       GLY B 172
                   CA
      MOTA
                                                                                        С
                                                         39.249
                                                                 1.00 51.80
                                       15.975
                                                67.066
             8697
                   С
                       GLY B 172
      ATOM
                                                                 1.00 54.56
                                                                                        0
                                                         39.524
                                       15.357
                                                68.102
                       GLY B 172
             8698
      ATOM
                   0
                                                                                        N
                                                         38.658
                                                                 1.00 48.83
                                        17.167
                                                67.063
                        SER B 173
             8699
                   N
      ATOM
                                                                                        С
                                                         38.259
                                                                 1.00 43.89
                                                68.288
                                        17.796
                        SER B 173
                   CA
35
             8701
      MOTA
                                                                                        C
                                                                  1.00 42.65
                                                68.557
                                                         39.113
                                        19.000
                        SER B 173
                   CB
      ATOM
             8703
                                                                                        0
                                                                 1.00 49.32
                                                         40.373
                                                69.033
                        SER B 173
                                        18.603
             8706
                   OG
      MOTA
                                                                  1.00 44.21
                                                         36.864
                                        18,297
                                                68.264
             8708
                   C
                        SER B 173
      ATOM
                                                                  1.00 45.21
                                                         36.273
                                                 67.207
                                        18.544
                        SER B 173
      MOTA
             8709
                   0
                                                         36.356
                                                                  1.00 43.20
                                                 69.476
                        MET B 174
                                        18.432
      MOTA
             8710
                   N
                                                                  1.00 43.58
                                                 69.725
                                                         35.148
                        MET B 174
                                        19.138
             8712
                   CA
      MOTA
                                                70.144
                                                         34.044
                                                                  1.00 43.84
                                        18.184
                        MET B 174
             8714
                   CB
      MOTA
                                                                  1.00 46.91
                                                70.650
                                                         32.883
                                        18.971
                        MET B 174
             8717
                    CG
      MOTA
                                                                  1.00 53.60
                                                         31.472
                                                 70.998
                                        18.074
                        MET B 174
             8720
                    SD
      ATOM
                                                                  1.00 56.75
                                                         31.872
                                                 72.553
                                        17.365
 45
      MOTA
             8721
                    CE
                        MET B 174
                                                                                        C
                                                         35.471
                                                                  1.00 45.69
                                        20.132
                                                 70.872
                        MET B 174.
                    С
      MOTA
             8725
                                                                                        O
                                                                  1.00 45.35
                                                72.028
                                                         35.575
                        MET B 174
                                        19.721
                   Ó
             8726
      MOTA
                                                                                        N
                                                                  1.00 41.84
                                                         35.650
                                        21.418
                                                 70.577
                    N
                        ILE B 175
             8727
      MOTA
                                                                                        C
                                                 71.663
                                                         35.853
                                                                  1.00 46.48
                                        22.376
                    CA
                        ILE B 175
              8729
      MOTA
                                       23.548
                                                                  1.00 47.95
                                                         36.811
                                                 71.295
                        ILE B 175
 50
              8731 -
                   CB
      MOTA
                                                                  1.00 46.56
                                                 70.444
                                                         37.989
                                        23.105
              8733
                    CG1
                        ILE B 175
      MOTA
                                                                  1.00 46.76
                                                         38.942
                                        22.250
                                                 71.153
                    CD1
                        ILE B 175
      MOTA
              8736
                                                                                         C
                                                                  1.00 45.43
                                        24.168
                                                 72.567
                                                         37.289
                   CG2 ILE B 175
      MOTA
              8740
                                                                                         C
                                                                  1.00 44.88
                                                 72.113
                                                         34.524
                        ILE B 175
                                        22.986
              8744
                    С
      MOTA
                                                         33.802
                                                                  1.00 48.63
                                                 71.333
                                        23.615
                        ILE B 175
              8745
                    0
 55
      ATOM
                                                 73.385
                                                          34.216
                                                                  1.00 51.15
                                        22.815
                        ILE B 176
              8746
                    N
      MOTA
                                                 73.942
                                                                  1.00 51.24
                                         23.223
                                                          32.922
              8748
                        ILE B 176
                    CA
      MOTA
                                                 74.980
                                                          32.470
                                                                  1.00 51.72
                                         22.198
              8750
                    CB
                        ILE B 176
      MOTA
                                                                  1.00 45.30
                                                 74.369
                                                          32.300
                                         20.833
                    CG1 ILE B 176
              8752
      MOTA
                                                                  1.00 49.64
                                                 74.362
                                                          30.860
                                         20.454
                    CD1 ILE B 176
              8755
 60
      MOTA
                                                 75.606
                                                          31.135
                                                                  1.00 53.65
                                         22.621
                    CG2 ILE B 176
              8759
       MOTA
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| | | | | | | | | | 1 00 | -n na . | | С |
|----------|-------|------|-----|--------------|----|--------|--------|--------|------|----------------|----------------------|-----|
| 5 | ATOM | 8763 | С | ILE B 176 | | 24.558 | 74.647 | | 1.00 | 50.93 52.76 | | o |
| | ATOM | | 0 | ILE B 176 | | 24.648 | 75.704 | | 1.00 | 53.67 | + : : - + | 'n |
| | ATOM | 8765 | N | GLY B 177 | | 25.584 | 74.065 | | | 52.15 | | Č |
| | MOTA | 8767 | CA | GLY B 177 | | 26.921 | 74.625 | 32.462 | 1.00 | | | Č |
| | MOTA | 8770 | С | GLY B 177 | | 27.839 | 74.139 | 33.561 | | | | ő |
| 10 | ATOM | | 0 | GLY B 177 | | 28.832 | 74.776 | 33.795 | | 52.76 | | N |
| .10 | ATOM | 8772 | N | GLY B 178 | | 27.538 | 73.029 | 34.224 | | 51.24 | | C |
| | ATOM | 8774 | CA | GLY B 178 | | 28.406 | 72.536 | 35.293 | | 51.26 | | c |
| | ATOM | 8777 | С | GLY B 178 | | 28.016 | 71.184 | 35.886 | 1.00 | 52.43 | | 0. |
| | ATOM | 8778 | 0 | GLY B 178 | | 27.068 | 70.577 | 35.440 | | 59.00 | | N |
| 15 | ATOM | 8779 | N | ILE B 179 | | 28.730 | 70.717 | 36.903 | | 50.07 | | C |
| 1.5 | ATOM | 8781 | CA | ILE B 179 | | 28.446 | | 37.512 | | 45.67 | | c |
| | ATOM | 8783 | СВ | ILE B 179 | | 29.610 | 68.519 | 37.252 | | 47.32 | | c |
| | ATOM | 8785 | | ILE B 179 | | 29.842 | 68.357 | 35.761 | | 49.07 | | c |
| • | ATOM | 8788 | CD1 | ILE B 179 | | 31.133 | 67.633 | 35.429 | | 45.35 | _ | C |
| 20 | ATOM | 8792 | | ILE B 179 | | 29.350 | 67.174 | 37.842 | | 48.87 | | |
| 20 | ATOM | 8796 | C | ILE B 179 | | 28.271 | 69.601 | 39.024 | | 46.31 | | C |
| | MOTA | 8797 | ō | ILE B 179 | | 29.115 | 70.203 | 39.691 | | 48.40 | | 0 |
| | MOTA | 8798 | N | ASP B 180 | | 27.199 | 69:060 | 39.581 | | 45.06 | | N |
| | ATOM | 8800 | | ASP B 180 | | 26.925 | 69.265 | 40.996 | | 46.20 | | C |
| 25 | ATOM | 8802 | СВ | ASP B 180 | | 25.489 | 69.733 | 41.193 | | 48.62 | | C |
| 23 | ATOM | 8805 | CG | ASP B 180 | | 25.183 | 70.143 | 42.644 | | 50.85 | | C |
| | ATOM | 8806 | | ASP B 180 | - | 25.059 | 71.353 | 42.922 | | 46.55 | | O O |
| | ATOM | 8807 | 002 | ASP B 180 | | 25.034 | 69.324 | 43.579 | | 57.84 | | 0 |
| | ATOM | 8808 | C. | ASP B 180 | | 27.169 | 68.037 | 41.828 | | 46.31 | | C |
| 30 | ATOM | 8809 | 0 | ASP B 180 | | 26.308 | 67.217 | 41.996 | 1.00 | 52.16 | | 0 |
| 30 | MOTA | 8810 | N | HIS B 181 | | 28.377 | 67.942 | 42.351 | | 51.89 | | N |
| | ATOM | 8812 | CA | HIS B 181 | | 28.831 | 66.897 | 43.277 | | 50.52 | | C |
| | ATOM | 8814 | CB | HIS B 181 | | 29.990 | 67.496 | 44.061 | | 50.18 | | C |
| | ATOM | 8817 | CG | HIS B 181 | | 31.190 | 67.731 | 43.220 | | 60.85 | | C |
| 35 | ATOM | 8818 | | HIS B 181 | | 32.309 | 68.400 | 43.673 | | 67.21 | | N |
| رد | ATOM | 8820 | | HIS B 181 | | 33.207 | 68.450 | 42.704 | | 70.69 | • | . с |
| | ATOM | 8822 | | 2 HIS B 181 | | 32.708 | 67.841 | 41.639 | | 75.54 | | . N |
| | ATOM | 8824 | | 2 HIS B 181 | | 31.447 | 67.381 | 41.936 | | 67.45 | | C |
| | ATOM | 8826 | C | HIS B 181 | | 27.858 | 66.226 | 44.276 | | 48.76 | | С |
| 40 | MOTA | 8827 | ō | HIS B 181 | | 28.090 | 65.086 | 44.671 | | 50.74 | | 0 |
| 70 | ATOM | 8828 | N | SER B 182 | | 26.797 | 66.891 | | | 47.39 | | N |
| | MOTA | 8830 | CA | SER B 182 | | 25.899 | 66.216 | 45.653 | | 47.06 | | C |
| | MOTA | 8832 | CB | SER B 182 | | 25.005 | 67.213 | 46.359 | | 44.50 | | C |
| | ATOM | 8835 | OG | | | 24.325 | 67.978 | | | 49.42 | | 0 |
| 45 | ATOM | 8837 | c | SER B 182 | | 25.041 | 65.202 | 44.909 | | 44.21 | | C |
| 43 | ATOM | 8838 | ō | SER B 182 | | 24.473 | 64.259 | 45.490 | | 42.19 | | . 0 |
| | MOTA | 8839 | N | LEU B 183 | | 24.941 | | | | 35.22 | | N |
| | MOTA | 8841 | CA | | | 24.017 | - · | | | 34.72 | | C |
| | ATOM | 8843 | СВ | | | 23.541 | 65.242 | 41.625 | | 37.22 | ٠ | C |
| 50 | | 8846 | CG | | | 23.060 | | | 1.00 | 35.27 | | C |
| JU | ATOM: | 8848 | CD | 1 LEU B 183 | | 22.723 | | 40.490 | | 35.13 | | ·C |
| • | MOTA | 8852 | | 2 LEU B 183 | | 21.845 | | | | 39.21 | | С |
| | ATOM | 8856 | | LEU B 183 | | 24.581 | | 42.659 | 1.0 | 0 34.54 | | С |
| | ATOM | | | LEU B 183 | | 23.893 | | | 1.0 | 0 32.68 | | 0 |
| | ATOM | 8857 | | TYR B 184 | ٠. | 25.814 | | | 1.0 | 0 40.53 | | N |
| 55 | MOTA | 8858 | | 101 | | 26.304 | | | | 0 40.17 | • | C |
| | MOTA | 8860 | | | | 26.806 | | | 1.0 | 0 42.80 | | С |
| | ATOM | 8862 | | 101 | • | 28.109 | | | | 0 39.74 | | С |
| | ATOM | 8865 | CC | 11K B 104 | | 28.111 | | | | 0 37.66 | | C |
| ~ | ATOM | 8866 | UL. | 11 TYR B 184 | | 29.253 | | | | 0 37.61 | | С |
| 60 | | 8868 | | | | 30.456 | | | | 0 47.41 | | С |
| | MOTA | 8870 | CZ | TIV D TOA | | 50.450 | | | | | | |

| _ | | 0071 | 011 | msen i | D 104 | 31.5 | 76 64.4 | 26 40.58 | 1 1.00 | 55.00 | | | 0 |
|------|------|--------------|------|--------|-------|-------|---------|----------|---------|---------|----|---|--------|
| 5 | ATOM | 8871 | | | B 184 | | | | | 43.25 | | | C. |
| | MOTA | 8873 | | | B 184 | 30.5 | | | | 41.71 | | | C |
| | MOTA | 8875 | | | B 184 | 29.3 | | | | 41.79 | | | c |
| | MOTA | 8877 | С | | B 184 | 27.4 | | | | 46.68 | | | ō |
| | MOTA | 8878 | 0 | | B 184 | 28.0 | | | | 43.21 | | | N |
| 10 | MOTA | 8879 | N | | B 185 | 27.6 | | | | 44.21 | | | C |
| | MOTA | 8881 | CA | | B 185 | 28.7 | | | | 44.37 | - | | c |
| : | MOTA | 8883 | CB | | B 185 | 28.1 | | | | 55.13 | | | ŏ |
| | MOTA | 8885. | | | B 185 | 27.2 | | | | | | | č |
| | ATOM | 8887 | CG2 | | B 185 | 27.2 | | | | 43.63 | | | c |
| 15 | MOTA | 8891 | С | | B 185 | 29.6 | | | | 43.25 | | | o |
| | MOTA | 8892 | 0 | | B 185 | 29.2 | | | | 41.22 | | | |
| | MOTA | 8893 | N | | В 186 | 30.9 | | | | 36.99 | | | N C |
| | ATOM | 8895 | CA | GLY | B 186 | 31.9 | | | | 37.15 | | | |
| • | ATOM | 8898 | C | | в 186 | 32.3 | | | | 39.52 | • | | C |
| 20 | ATOM | 8899 | .0 | GLY | в 186 | 31.9 | | | | 41.98 | | | 0 |
| | ATOM | 8900 | N | SER | B 187 | 33.1 | 06 57.6 | | _ | 41.91 | | | N |
| | ATOM | 8902 | CA | SER | B 187 | 33.7 | 02 58.4 | | | 43.54 | | | С |
| | ATOM | 8904 | СВ | SER | в 187 | 35.1 | 32 57.9 | 57 39.93 | | 49.17 | | | С |
| | ATOM | 8907 | OG | | в 187 | | | | | 51.70 | | | 0 |
| 25 | ATOM | 8909 | C | | в 187 | 32.9 | 06 58.5 | 52 38.9 | | 38.74 | | | С |
| 23 | ATOM | 8910 | ō | | в 187 | 32.1 | | | 77 1.00 | 44.27 | | | 0 |
| | ATOM | 8911 | N | | B 188 | | 54 59.6 | 49 38.23 | 36 1.00 | 36.60 | | | N |
| | ATOM | 8913 | CA | | В 188 | | 51 59.7 | 79 36.9 | 08 1.00 | 36.77 | | | С |
| | ATOM | 8915 | СВ | | B 188 | | | | 30 1.00 | 29.29 | | | . C |
| 30 | ATOM | 8918 | CG | | В 188 | | | 59 36.6 | 95 1.00 | 26.22 | | | С |
| . 50 | ATOM | 8920 | | | B 188 | | | | 19 1.00 | 31.52 | | • | С |
| | ATOM | 8924 | | | B 188 | | | | | 28.00 | | | С |
| | MOTA | 8928 | C | | B 188 | | | | | 37.01 | | | C |
| | | 8929 | Ö | | B 188 | | | | | 42.16 | ٠. | | 0. |
| 25 | MOTA | 8930 | N | | B 189 | | | | | 44.14 | | | N |
| 35 | MOTA | | CA | | B 189 | | | | | 40.20 | | | С |
| | MOTA | 8932 8934 | CB | | B 189 | | | | | 42.63 | | | С |
| | ATOM | | CG | | В 189 | | | | | 44.06 | | | С |
| | ATOM | 8937 | CD1 | | B 189 | | | | | 38.39 | | | C |
| 40 | ATOM | 8938 | | | B 189 | | | | | 45.18 | | | N |
| 40 | MOTA | 8940 | | | B 189 | | | | | 44.17 | | | С |
| | MOTA | 8942 | | | B 189 | | | | | 44.91 | | | С |
| | MOTA | 8943 | | | B 189 | | | | | 53.36 | • | | C |
| | MOTA | 8944 | | | | | | | | 52.20 | | | С |
| 40 | MOTA | 8946 | | | B 189 | | | | | 50.78 | | | С |
| 45 | ATOM | 8948 | | | B 189 | | | | | 50.20 | | | С |
| | MOTA | 8950 | | | B 189 | | | | - | 43.79 | | | C |
| | MOTA | 8952 | C | | B 189 | | | | | 46.26 | | | ō |
| | MOTA | 8953 | 0 | | В 189 | | | | | 42.68 | | | N |
| | MOTA | 8954 | N | | B 190 | | | | | 39.84 | | | C |
| 50 | MOTA | 8956 | CA | | B 190 | | | | | | | | č |
| | MOTA | 8958 | CB | | В 190 | | 052 60. | | | 36.42 | | | c |
| • | MOTA | 8961 | CG | | В 190 | | 685 61. | | | 33.81 | | | C |
| • | ATOM | 8962 | CD1 | TYR | B 190 | | | 624 32.1 | | 37.07 | | | |
| | ATOM | 8964 | CE 1 | TYR | B 19 | | | 703 32.9 | | 0 42.72 | | | C |
| 55 | ATOM | 8966 | CZ | TYR | B 19 | | | 450 32.5 | | 0 45.10 | | | C |
| | ATOM | 8967 | ÓН | | В 19 | | | 565 33.3 | | 0 53.55 | | | .0 |
| | ATOM | 8969 | CE2 | YYR | B 19 | | | 102 31.5 | | 0 30.96 | | | C |
| | ATOM | 8971 | | | B 19 | 0 32. | | 043 30.7 | | 0 33.25 | | | C |
| | ATOM | 8973 | | | В 19 | | | 066 28.9 | | 0 38.96 | | | C |
| 60 | ATOM | 8974 | | | В 19 | 0 34. | | 748 28. | | 0 51.45 | | | 0 |
| | ATOM | 8975 | | | В 19 | | 312 57. | 822 28.2 | 210 1.0 | 0 47.13 | | | N |
| | | | | | | | | | | | | | |

| | | | | | | | | | | | | | _ |
|-------------|------|-------|------|---------|-------|----|--------|--------|------------------|------|---------|------|--------|
| 5 | ATOM | 8977 | CA | THR B | 191 | | 32.398 | 57.242 | 26.864 26.566 | | 47.27 | 47.7 | C C |
| • | ATOM | 8979 | | | 191 | ٠. | | | | 1.00 | 50.31 | | ŏ |
| | ATOM | 8981 | OG1 | THR B | | | 31.383 | 55.461 | 25.550 | | | | c |
| | ATOM | 8983 | CG2 | | | | 30.100 | 57.286 | 25.966 | | 48.46 | | c |
| | ATOM | 8987 | С | THR .B | 191 | | 32.464 | 58.404 | 25.872 | | 51.71 | | o |
| 10 | ATOM | 8988 | 0 | THR B | 191 | | 31.924 | 59.462 | 26.120 | | 56.58 | | N |
| | MOTA | 8989 | N | PRO B | 192 | | 33.116 | 58.236 | 24.741 | | 54.66 | | C |
| | MOTA | 8990 | CA | PRO B | 192 | | 33.183 | 59.339 | 23.783 | 1.00 | 53.51 | | C. |
| | ATOM | 8992 | CB | PRO B | 192 | | 34.249 | 58.903 | 22.788 | | 53.85 | | C |
| | ATOM | 8995 | CG | PRO B | 192 | | 34.716 | 57.512 | 23.244 | | 56.15 | · | c |
| 15 | ATOM | 8998 | CD | PRO B | | | 33.802 | 57.022 | 24.282 | | 54.11 | | C. |
| | MOTA | 9001 | С | PRO B | 192 | | 31.875 | 59.435 | 23.058 | | 53.29 | | 0 |
| | ATOM | 9002 | 0 | PRO B | | | 31.105 | 58.500 | 23.175 | | 48.91 | | И |
| | ATOM | 9003 | N | ILE B | 193 | | 31.654 | 60.547 | 22.351 | | 53.07 | | C |
| • | ATOM | 9005 | CA | ILE B | 193 | | 30.506 | 60.753 | 21.490 | | 47.51 | | c |
| 20 . | MOTA | 9007 | CB | ILE B | 193 | | 29.967 | 62.149 | 21.619 | | 53.03 | | C |
| 20. | MOTA | 9009 | | ILE B | | | 29.103 | 62.310 | 22.871 | | 53.04 | | |
| | ATOM | 9012 | CD1 | ILE B | 193 | | 28.952 | 63.742 | 23.319 | | 53.15 | | C |
| | ATOM | 9016 | | ILE B | | | 29.109 | 62.457 | 20.421 | | 53.72 | | C |
| | ATOM | 9020 | С | ILE B | 193 | | 31.029 | 60.603 | 20.091 | | 50.01 | | C |
| 25 | ATOM | 9021 | 0 | ILE B | | | 31.857 | 61.413 | 19.615 | | 45.74 | | 0 |
| 23 | ATOM | 9022 | N | ARG B | 194 | | 30.519 | 59.566 | | | 49.20 | | N |
| | ATOM | 9024 | CA | ARG B | | | 30.954 | 59.093 | 18.139 | | 48.45 | | C |
| | ATOM | 9026 | СВ | ARG B | | | 30.161 | 57.826 | 17.861 | | 46.41 | | Ċ |
| | ATOM | 9029 | CG | ARG B | | | 30.797 | 56.851 | 16.901 | | 47.20 | | C |
| 30 | ATOM | 9032 | CD | ARG B | | • | 29.735 | 56.067 | 16.153 | | 43.61 | * | C |
| 5,0 | ATOM | 9035 | NE | ARG B | | | 30.326 | 55.148 | 15.205 | | 44.33 | | N |
| | ATOM | 9037 | CZ | ARG B | | | 29.624 | 54.477 | 14.301 | | 45.08 | | C. |
| | ATOM | 9038 | | ARG E | | | 28.331 | 54.639 | 14.241 | | 42.10 | | N |
| | ATOM | 9041 | | ARG E | | | 30.207 | 53.647 | 13.452 | | 44.38 | | N |
| 35 | ATOM | 9044 | С | ARG E | | | 30.740 | 60.071 | 16.978 | | 55.22 | | Ċ |
| 33 | ATOM | 9045 | 0 | ARG E | | | 31.503 | 60.047 | 15.987 | | 56.72 | | 0 |
| | ATOM | 9046 | N. | | | | 29.696 | 60.906 | 17.113 | | 57.00 | | N |
| | MOTA | 9048 | CA | ARG E | 3 195 | | 29.244 | 61.865 | | | 53.97 | | C |
| | ATOM | 9050 | СВ | | 3 195 | | 28.412 | 61.171 | | | 55.76 | | C |
| 40 | ATOM | 9053 | CG | - | 3 195 | | 28.550 | 61.762 | | | 60.64 | | C |
| -10 | ATOM | 9056 | CD | | в 195 | | 27.234 | 61.923 | | | 60.09 | | C |
| | ATOM | 9059 | NE | | B 195 | | 26.847 | 60.696 | | | 64.82 | | N |
| | ATOM | 9061 | CZ | | B 195 | | 26.074 | 60.632 | | | 66.70 | | C |
| • | ATOM | 9062 | | L ARG I | | | 25.572 | 61.735 | | | 66.60 | | N |
| 45 | ATOM | 9065 | | 2 ARG | | | 25.799 | 59.444 | | | 0 67.97 | | N |
| 1.5 | MOTA | 9068 | С | | В 195 | | 28.326 | | | | 0 52.68 | | C |
| | ATOM | 9069 | 0 | ARG 1 | В 195 | | 27.499 | | 17.605 | | 0 48.21 | - | 0 |
| | ATOM | .9070 | N | | в 196 | | 28.455 | 64.127 | | | 0 48.78 | | N. |
| | MOTA | 9072 | | | В 196 | | 27.569 | | 17.046 | 1.0 | 0 48.32 | | C |
| 50 | MOTA | 9074 | | | В 196 | | 28.199 | 66.421 | 17.091 | | 0 47.83 | | C |
| 50 | ATOM | 9077 | | | B 196 | | 29.399 | 66.401 | 17.960 | | 0 48.63 | | C |
| | MOTA | 9080 | | | B 196 | | 30.197 | | | | 0 47.85 | | C. |
| | MOTA | 9081 | | 1 GLU | | | 31.098 | | 16.899 | | 0 45.46 | | 0 |
| | MOTA | 9082 | | 2 GLU | | | 29.909 | | | 1.0 | 0 49.47 | | . 0 |
| 55 | | 9083 | | | B 196 | | 26.332 | | | | 0 48.04 | | С |
|)) | | 9084 | | | B 196 | | 26.225 | | | | 0.51.46 | | 0 |
| | ATOM | 9085 | | | B 197 | | 25.402 | | | | 0 43.41 | | N |
| | MOTA | 9087 | | | B 197 | | 24.115 | | | | 0 42.70 | | С |
| | MOTA | 9089 | | | B 197 | | 24.013 | | 2 14.546 | | 0 42.18 | | С |
| 60 | ATOM | 9092 | | | B 197 | | 24.166 | | | | 0 44.56 | | С |
| ŅΟ | | 9093 | | 1 TRP | | | 25.015 | | | | 0 48.17 | | C |
| | MOTA | 909. | , 00 | | | | | | | | | | |

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59.961 15.166
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                     CE1 TYR B 198
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20
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                         TYR B 198
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                     CD2 TYR B 198
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                         TYR B 198
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                                                    62.908
                                                             18.991
                          TYR B 198
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                                                                                               C.
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                         TYR B 199
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                     CG
      ATOM
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B 200 20
B 200 26
GLU B 200 26
GLU B 200 26.
GLU B 200 27.8
GLU B 201 26.70
C GLU B 201 27.77
CB VAL B 201 27.515
CG1 VAL B 201 27.484
CG2 VAL B 201 27.78
VAL B 201 27.78
VAL B 201 26.230
C VAL B 201 27.78
VAL B 201 26.230
C VAL B 201 26
ILE B 202
ILE B 202
ILE B 202
ILE B 202
ILE B 207
ILE B
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                         GLU B 200
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                                                                                               С
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      MOTA
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      MOTA
               9162
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                                                                       1.00 50.91
               9163
      MOTA
                                                                                               С
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                                                                       1.00 46.93
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21.021
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                                                                       1.00 52.84
      ATOM
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                                                              23.383
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                                                              20.431
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               9195
                          ILE B 202
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                                                                       1.00 42.02
                     С
 60
               9199
      MOTA
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                          ILE B 202
                                           29.706 51.788 23.359
                                                                       1.00 44.16
               9200
      MOTA
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| 5 | ATOM | 9201 | N | ILE B | 203 | 28.429 | 50.423 | 22.252 | | 42.56 | | N |
|------|-------|------|-------|-------|----------------|--------|--------|------------------|------|---------|----|-------|
| | ATOM | 9203 | | ILE E | | 28.259 | 49.497 | 23.327 | | 45.31 | | С |
| | ATOM | 9205 | | ILE E | | 26.823 | 49.150 | 23.567 | | 43.41 | | С |
| | ATOM | 9207 | | ILE E | | 26.040 | 50.325 | 24.088 | | 41.62 | | С |
| | ATOM | 9210 | | ILE E | | 24.600 | 49.972 | 24.158 | 1.00 | 42.16 | | С |
| 10 | ATOM | 9214 | | | 3 203 | 26.780 | 48.073 | 24.599 | 1.00 | 44.28 | | С |
| 10 | ATOM | 9218 | | ILE E | | 28.888 | 48.250 | 22.866 | | 49.14 | ٠. | C |
| | MOTA | 9219 | | ILE E | | 28.537 | 47.712 | 21.806 | 1.00 | 47.82 | | 0 |
| | ATOM | 9220 | | | 3 204 | 29.782 | 47.762 | 23.696 | 1.00 | 49.32 | | N |
| | | 9222 | | VAL E | | 30.610 | 46.689 | 23.294 | 1.00 | 48.88 | | C |
| 15 | MOTA | 9224 | | VAL E | | 31.996 | 47.004 | 23.720 | 1.00 | 45.35 | | С |
| 15 | MOTA | 9226 | | VAL E | | 32.441 | 48.273 | 23.012 | 1.00 | 49.69 | | C. |
| | MOTA | 9230 | | | 3 204 | 32.055 | 47.203 | 25.163 | | 44.93 | | С |
| | MOTA | 9234 | | | 3 204 | 30.179 | 45.382 | 23.866 | 1.00 | 51.35 | | С |
| • | MOTA | | | | 3 204 | 30.565 | 44.349 | 23.337 | | 57.30 | | О |
| 20 | MOTA | 9235 | | | 3 205 | 29.392 | 45.397 | 24.941 | | 50.88 | | N |
| 20 | ATOM | 9236 | | | 3 205 B 205 | 29.044 | 44.122 | 25.568 | | 52.74 | | С |
| | ATOM. | 9238 | | | B 205 | 30.299 | 43.498 | 26.174 | | 52.53 | | С |
| | MOTA | 9240 | | | B 205 | 30.064 | 42.536 | 27.318 | | 54.44 | | С |
| | MOTA | 9243 | | | B 205 | 31.354 | 41.863 | 27.754 | | 56.13 | | С |
| ~- | ATOM | 9246 | | | | 31.296 | 41.266 | 29.087 | | 59.87 | | N |
| . 25 | MOTA | 9249 | NE | | B 205 | 31.742 | 40.048 | 29.378 | | 59.78 | | C. |
| | ATOM | 9251 | CZ | | B 205 | 32.275 | 39.296 | 28.429 | | 58.07 | | N |
| | ATOM | 9252 | | | B 205 | 32.273 | 39.585 | 30.618 | | 61.85 | | N |
| | MOTA | 9255 | | | B 205 | | 44.177 | 26.605 | | 50.44 | | C |
| •• | ATOM | 9258 | C. | | B 205 | 27.953 | 44.177 | 27.512 | | 60.70 | | ō |
| 30 | MOTA | 9259 | 0 | | B 205 | 28.004 | | 26.455 | | 48.83 | | N |
| | MOTA | 9260 | N | | B 206 | 26.972 | 43.298 | 27.373 | | 48.98 | | Ċ |
| | ATOM | 9262 | CA | | B 206 | 25.846 | 43.189 | 26.609 | | 47.56 | | Č |
| | MOTA | 9264 | CB | | В 206 | 24.544 | 43.113 | 27.571 | | 51.41 | | Č |
| | MOTA | 9266 | | | В 206 | 23.429 | 42.948 | | | 47.81 | | c |
| · 35 | MOTA | 9270 | | | B 206 | 24.310 | 44.358 | 28.204 | | 49.62 | | Č |
| | ATOM | 9274 | С | | В 206 | 25.931 | 41.888 | | | 51.17 | | ŏ |
| | ATOM | 9275 | 0 | | В 206 | 26.324 | 40.839 | 27.707 29.466 | | 48.53 | | N |
| | MOTA | 9276 | N | | В 207 | 25.549 | 41.972 | | | 50.25 | | C |
| | MOTA | 9278 | CA | | В 207 | 25.511 | 40.846 | 30.346 | | 50.16 | | c |
| 40 | MOTA | 9280 | CB | | В 207 | 26.588 | 40.933 | 31.415 | | 49.74 | | č |
| | MOTA | 9283 | CG | | В 207 | 27.966 | 40.533 | 30.976 | | 49.93 | | č |
| | MOTA | 9286 | CD | | В 207 | 28.971 | 40.942 | 32.003 | | 53.30 | | Ö |
| | MOTA | 9287 | | | В 207 | 28.551 | 41.333 | 33.115 | | 51.43 | | ő |
| | MOTA | 9288 | | | В 207 | 30.168 | 40.887 | 31.697 | | | | c |
| 45 | ATOM | 9289 | С | | В 207 | 24.194 | | 31.063 | | 53.82 | | Ö |
| • | ATOM | 9290 | 0 | | В 207 | 23.625 | | 31.314 | - | 53.60 | | ·N |
| | MOTA | 9291 | N | | В 208 | 23.715 | 39.664 | 31.408 | | 56.66 | | C |
| | MOTA | 9293 | CA | | B 208 | 22.535 | | 32.224 | | 54.83 | | |
| | MOTA | 9295 | CB | | B 208 | 21.422 | | 31.434 | | 55.18 | | C |
| 50 | MOTA | 9297 | · CG1 | ILE | B 208 | 21.118 | | 30.212 | | 56.27 | | C |
| | MOTA | 9300 | CD1 | ILE | B 208 | 20.393 | | 30.503 | | 0 49.77 | | . C |
| | MOTA | 9304 | CG2 | ILE | B 208 | 20.205 | | | | 0 57.22 | | C |
| | ATOM | 9308 | С | ILE | B 208 | 22.955 | | 33,429 | | 0 57.88 | | C |
| | ATOM | 9309 | . 0 | ILE | B 208 | 23.347 | | 33.302 | | 0 57.17 | | 0 |
| 55 | ATOM | 9310 | N | ASN | B 209 | 22.883 | 39.337 | 34.603 | | 0 54.93 | | N |
| · | ATOM | 9312 | CA | | B 209 | 23.319 | | 35.835 | | 0 56.25 | | C |
| | ATOM | 9314 | СВ | | B 209 | 22.270 | 37.722 | 36.372 | | 0 54.61 | | C |
| | ATOM | 9317 | CG | | B. 209 | 21.639 | 38.210 | 37.663 | | 0 55.46 | | С |
| | ATOM | 9318 | | | В 209 | 21.992 | | 38.187 | 1.0 | 0 50.67 | | 0 |
| 60 | | 9319 | | | В 209 | 20,695 | | 38.189 | 1.0 | 0 53.95 | | N |
| 00 | ATOM | 9322 | | | B 209 | 24.668 | 38.015 | 35.668 | 1.0 | 0 52.94 | | С |
| | MION | | - | | | | | | | | • | |

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36.076 1.00 47.18
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            9343 NE2 GLN B 211
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                                                                                   С
                      GLN B 211
                                     25.986
                                             36.886
                                                      30.522
            9346 C
     MOTA
                                    24.946
                                             37.452
                                                      30.180
                                                              1.00 54.93
                                                                                   0
            9347 0
                      GLN B 211
     MOTA
                                                              1.00 52.76
                                             36.852
                                                                                   N
            9348
                 N
                      ASP B 212
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                                                      28.466
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                                                                                   С
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                      ASP B 212
     MOTA
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                      ASP B 212
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                  OD2 ASP B 212
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                                                              1.00 61.19
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                                                      26.738
                                                              1.00 62.11
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                      LEU B 213
     ATOM
            9360
                  N
                                     24.673 37.937
                                                      25.688
                                                              1.00 61.19
                                                                                    C
            9362
                      LEU B 213
     MOTA
                  CA
                                                              1.00 62.39
                      LEU B 213
                                     24.155 39.306
                                                      25.248
                                                                                   C
     MOTA
            9364
                  CB
                                             39.359
                                                              1.00 58.53
                                     22.628
                                                      25.155
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     ATOM
            9367
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                      LEU B 213
                                                              1.00 57.55
                                                                                    C
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                                             38.183
                                                      25.895
                  CD1 LEU B 213
            9369
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                                                                                    С
                                     22.041
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                                                      25.697
     MOTA
            9373
                  CD2 LEU B 213
                                                              1.00 63.18
                                                                                    С
                                     25.319
                                              37.210
                                                      24.534
     ATOM
            9377
                  С
                      LEU B 213
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                                                      23.794
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                                                                                    0
                      LEU B 213
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            9378
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                                                                                    N
35
                      LYS B 214
     MOTA
            9379
                  N
                                                      23.539
                      LYS B 214
                                                              1.00 70.91
                                     27.466 36.603
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                  CA
                                                              1.00 69.78
                                     27.309
                                             35.139
                                                      23.941
                      LYS B 214
     MOTA
            9383
                  CB
                                                              1.00 71.78
                                                                                    С
                                                      23.410
                      LYS B 214
                                     28.397
                                             34.242
            9386
                  CG
     MOTA
                                                              1.00 72.93
                                                                                    С
                                      28.266 32.838
                                                      23.992
            9389
                      LYS B 214
     MOTA
                  CD
                                     28.927
                                             31.796
                                                      23.116
                                                              1.00 70.34
                                                                                    С
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40
     MOTA
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                                  27.903 31.146
                                                              1.00 64.34
                                                                                   N
                      LYS B 214
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            9395
     ATOM
                  NZ
                      LYS B 214
                                      27.143 36.780
                                                      22.072
                                                              1.00 73.22
                                                                                    C
            9399
                  C
     ATOM
                                   27.246
                                              35.850
                                                              1.00 66.62
                                                                                    0
                                                      21.251
            9400
                  0
                      LYS B 214
     MOTA
                                                              1.00 75.18
                                                                                    N
     MOTA
                      MET B 215
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                                              38.011
                                                      21.774
            9401 N
                                                              1.00 73.26 .
                                                                                    C
                                                      20.440
45
            9403
                      MET B 215
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                                              38.407
     MOTA
                  CA
                                                              1.00 72.49
                      MET B 215
                                      25.290
                                              39.408
                                                      20.449
                                                                                    C
            9405
                  CB
     MOTA
                                      23.998
                                              38.728
                                                      20.268
                                                              1.00 72.86
                                                                                    C
                      MET B 215
     MOTA
            9408
                  ĊG
                                      22.683 39.755
                                                      20.640
                                                              1.00 75.68
            9411
                      MET B 215
     MOTA
                  SD
                                      21.602
                                              39.194
                                                      19.427
                                                              1.00 75.77
                                                                                    C
                      MET B 215
     MOTA
            9412
                  CE
                                              39.092
                                                      19.959
                                                              1.00 73.98
                                                                                    С
50
     ATOM
            9416
                      MET B 215
                                      27.642
                  С
                                                              1.00 71.14
                                                                                    0
                                      28.518
                                              39.477
                                                      20.760
            9417
                      MET B 215
     MOTA
                  0
                                                      18.644
                                                              1.00 72.78
                                                                                   N
                      ASP B 216
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                                              39.237
     MOTA
            9418
                  N
                                                      18.037
                                                              1.00 71.14
                                                                                    C
                      ASP B 216
                                      28.719
                                              40.037
     MOTA
            9420
                  CA
                                                      16.540
                                                                                    C
                                    28.767
                                             39.744
                                                              1.00 71.31
     ATOM
            9422
                  CB
                      ASP B 216
                                                      15.771
                                                              1.00 74.43
                                                                                    C
                      ASP B 216
                                      29.577
                                             40.749
55
            9425
                  CG
     ATOM
                                              41.594
                                                      16.394
                                                               1.00 80.47
                                                                                    0
                                      30.271
     MOTA
            9426
                  OD1 ASP B 216
                                                      14.524
                  OD2 ASP B 216
                                      29.584
                                              40.763
                                                              1.00 72.09
                                                                                    0
            9427
     MOTA
                                                      18.401
                                                               1.00 68.29
                      ASP B 216
                                      28.186
                                              41.415
     MOTA
            9428
                  С
                                              41.655
                                                      18.318
                                                               1.00 62.61
            9429
                      ASP B 216
                                      26.983
     MOTA
                  0
                      CYS B 217
                                      29.061
                                              42.308
                                                      18.831
                                                               1.00 68.51
     MOTA
            9430
                  N
                      CYS B 217
                                      28.625
                                              43.609
                                                      19.316 1.00 68.58
     MOTA
             9432
                  CA
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| _ | | 0434 | CD | CYS E | 217 | | 29.795 | 44.285 | 19.994 | 1.00 | 68.63 | | | | C |
|----|------|------|-----|-------|-------|----------|--------|------------------|------------------|-------|---------|---|---|-----|-----|
| 5 | MOTA | | CB | CYS E | | | | 44.299 | 18.997 | | 74.46 | | | | S. |
| | MOTA | • | SG | CYS E | | | 28.007 | 44.565 | 18.282 | 1.00 | 70.29 | | | (| C . |
| | MOTA | | C | CYS E | | | 27.287 | 45.509 | 18.640 | 1.00 | 68.93 | | | (| 0 |
| | MOTA | | 0 | LYS E | | | 28.244 | 44.334 | 17.002 | | 71.63 | | | | N |
| | ATOM | • • | N | | | | 27.750 | | 16.014 | | 70.37 | | | . (| С |
| 10 | MOTA | | CA | LYS E | | | 28.259 | 44.933 | 14.611 | 1.00 | 71.99 | | | (| С |
| | MOTA | 9444 | CB | LYS E | | | | 46.076 | 13.943 | | 76.53 | | | (| С |
| | MOTA | 9447 | CG | LYS I | | | 29.041 | 45.730 | 12.496 | | 80.60 | | | 4 | С |
| | MOTA | 9450 | | LYS I | | | 29.452 | 46.715 | 11.896 | | 83.08 | | | | С |
| | MOTA | 9453 | CE | LYS I | | | 30.493 | 46.715 | 12.763 | | 84.11 | | | | N |
| 15 | ATOM | 9456 | NZ | | B 218 | | 31.690 | | 16.063 | | 66.79 | | | | C |
| | ATOM | 9460 | С | | B 218 | | 26.229 | 45.322 | 15.509 | | 63.62 | | | | 0 |
| | MOTA | 9461 | 0 | | B 218 | | 25.578 | 46.202 44.352 | | | 64.08 | | | | N |
| | MOTA | 9462 | N | | В 219 | | 25.659 | | 16.800 | | 66.34 | | | | С |
| • | ATOM | 9464 | CA | | B 219 | | 24.222 | 44.244 | | | 69.58 | | | | C |
| 20 | ATOM | 9466 | CB | | B 219 | | 23.839 | 42.798 | 17.059 16.166 | | 71.88 | | | | С |
| | MOTA | 9469 | CG | | B 219 | | 24.551 | 41.798 | | | 78.40 | | | | Č |
| | MOTA | 9472 | CD | | B 219 | | 23.800 | 41.529 | 14.875 | | 72.86 | | | | ō |
| | MOTA | 9473 | OE1 | GLU | в 219 | | 22.637 | 42.002 | 14.721 | | 85.55 | | | | ō |
| | ATOM | 9474 | OE2 | GLU | B 219 | | 24.389 | 40.835 | 14.009 | | 65.05 | | | | c |
| 25 | ATOM | 9475 | С | | B 219 | | 23.691 | 45.065 | 17.931 | | | | | | 0 |
| 20 | ATOM | 9476 | 0 | GLU | B 219 | | 22.528 | 45.438 | 17.961 | | 63.97 | | | • | N |
| | ATOM | 9477 | N | TYR | B 220 | | 24.550 | 45.342 | 18.888 | | 65.15 | | | | C |
| | ATOM | 9479 | CA | TYR | B 220 | | 24.080 | 45.993 | 20.070 | | 62.09 | | | | c |
| | ATOM | 9481 | CB | TYR | B 220 | | 25.134 | 45.900 | 21.179 | | 62.12 | | | | c |
| 30 | ATOM | 9484 | CG | | B 220 | | 25.409 | 44.536 | 21.845 | | 56.86 | | | | C |
| 50 | ATOM | 9485 | CD1 | | B 220 | | 26.716 | 44.158 | 22.123 | | 60.11 | | | | C |
| | ATOM | 9487 | | | B 220 | | 27.019 | 42.952 | 22.738 | | 59.02 | | | | C |
| | ATOM | 9489 | CZ | | B 220 | | 26.013 | 42.097 | 23.090 | | 60.03 | | | | |
| | MOTA | 9490 | ОН | | В 220 | | 26.387 | 40.915 | 23.694 | | 65.94 | | | | 0 |
| 35 | ATOM | 9492 | | | B 220 | | 24.689 | 42.438 | 22.840 | | 57.10 | | | | C |
| 33 | ATOM | 9494 | | | в 220 | | 24.396 | 43.658 | 22.216 | | 55.80 | | | | С |
| | ATOM | 9496 | C | | B 220 | | 23.817 | 47.430 | 19.628 | | 61.17 | | | | C |
| | ATOM | 9497 | ō | | В 220 | | 22.944 | 48.103 | 20.158 | | 64.67 | | | | 0 |
| | ATOM | 9498 | N | | B 221 | | 24.569 | 47.880 | 18.628 | | 59.63 | | | | N |
| 40 | ATOM | 9500 | CA | | B 221 | | 24.486 | 49.244 | 18.114 | | 56.38 | | | | C |
| ΨŲ | ATOM | 9502 | CB | | B 221 | | 25.865 | 49.780 | 18.037 | | 53.93 | | | | C |
| | ATOM | 9505 | CG | | B 221 | | 26.510 | 49.843 | 19.322 | | 51.48 | | | | С |
| | | 9506 | | N2A I | B 221 | | 26.001 | 50.434 | 20.257 | | 51.50 | | | | 0 |
| | MOTA | 9507 | ND. | M A A | B 221 | | 27.686 | 49.245 | 19.405 | | 56.63 | | | | N |
| 45 | MOTA | 9510 | C | ASN | B 221 | • | 23.971 | | | .1.00 | 58.77 | | | | С |
| 43 | MOTA | 9511 | | ASN | В 221 | | 24.232 | | | | 59.98 | | | | 0 |
| | ATOM | 9512 | N | | B 222 | | 23.235 | | | 1.00 | 59.18 | | | | N |
| | ATOM | 9514 | CA | | B 222 | | 22.870 | | 14.998 | 1.00 | 60.10 | | | • | C |
| | ATOM | | | WAD. | B 222 | , | 22.291 | | • | 1.0 | 0 64.25 | | | | ·C |
| 50 | ATOM | 9516 | CB | | B 222 | | 21.579 | | | | 0 65.11 | | | | · C |
| 50 | MOTA | 9519 | CG | | B 222 | | 22.008 | , | | | 0 67.45 | | | | С |
| | ATOM | 9520 | | | | | 21.356 | | | | 0 68.44 | | | | С |
| | ATOM | 9522 | | T TIK | B 222 | | 20.261 | | | | 0 68.04 | | | | С |
| | MOTA | 9524 | CZ | | B 222 | | 19.605 | | | | 0 72.86 | | | | 0 |
| | MOTA | 9525 | OH | | В 222 | | 19.814 | | | | 0 65.98 | | | | С |
| 55 | ATOM | 9527 | CE | Z TYR | B 222 | <u>د</u> | | | | | 0 66.41 | | | | С |
| | MOTA | 9529 | | Z TYR | B 22 | <u>د</u> | 20.470 | | | | 0 57.69 | | | | С |
| | MOTA | 9531 | C | | В 22 | | 21.922 | | | | 0 57.52 | | | | 0 |
| | MOTA | 9532 | | TYR | B 22 | ۷ | 20.737 | | | | 0 58.59 | | | | N |
| | MOTA | 9533 | | ASF | В 22 | <u>ა</u> | 22.571 | | | | 0 57.20 | | • | | C |
| 60 | MOTA | 9535 | | ASE | В 22 | 3 | 22.058 | | | | 0 62.18 | | | | · Č |
| | ATOM | 9537 | CE | ASE | В 22 | 3 | 20.51 | l 51.26 | 4 TO.T.C | . 1.0 | 02.10 | • | | | |
| | | | | | | | | | | | | | | | |

| 5 | ATOM | 9540 | CG · | ASP B 223 | 19.929 | 52.514 | 12.350 | 1.00 65.70 | | | С |
|-----|-------|-------|------|-----------|------------|--------|--------|------------|-----|---|------|
| | ATOM | 9541 | | ASP B 223 | 19.045 | 53.192 | 12.919 | 1.00 72.63 | | | 0 |
| | ATOM | 9542 | | ASP B 223 | 20.243 | 52.884 | 11.172 | 1.00 60.60 | | | 0 |
| | | 9543 | | ASP B 223 | 22.694 | 52.313 | 14.142 | 1.00 52.54 | | | С |
| | MOTA | 9544 | | ASP B 223 | 23.514 | 53.049 | 13.659 | 1.00 53.53 | | | 0 |
| 10 | MOTA | _ | | LYS B 224 | 22.364 | 52.357 | 15.416 | 1.00 55.48 | | | N |
| 10 | MOTA | 9545 | | | 22.905 | 53.373 | 16.312 | 1.00 53.90 | | | С |
| | MOTA | 9547 | | LYS B 224 | | | | 1.00 55.04 | | | č |
| | MOTA | 9549 | | LYS B 224 | 22.306 | 54.743 | 16.002 | 1.00 52.13 | | | Ċ |
| | MOTA | 9552 | CG | LYS B 224 | 20.794 | 54.865 | 16.179 | | | | c |
| : | MOTA | 9555 | | LYS B 224 | 20.386 | 56.306 | 15.817 | 1.00 47.46 | | | c |
| 15 | ATOM | 9558 | CE | LYS B 224 | 18.962 | 56.435 | 15.312 | 1.00 47.23 | | | |
| | ATOM | 9561 | NZ | LYS B 224 | 18.922 | 56.181 | 13.825 | 1.00 47.81 | | | N |
| | MOTA | 9565 | С | LYS B 224 | 22.640 | 53.044 | 17.752 | 1.00 55.74 | : | | С |
| | ATOM | 9566 | 0 | LYS B 224 | 22.165 | 51.982 | 18.073 | 1.00 56.88 | | | 0 |
| | ATOM | 9567 | N | SER B 225 | 22.974 | 53.966 | 18.632 | 1.00 59.75 | | | N |
| 20 | MOTA | 9569 | CA | SER B 225 | 22.735 | 53.775 | 20.046 | 1.00 58.65 | | | С |
| 20 | | 9571 | CB | SER B 225 | 23.820 | 52.902 | 20.666 | 1.00 58.31 | | | С |
| | ATOM | | | SER B 225 | 23.410 | 51.542 | 20.653 | 1.00 64.32 | | | 0 |
| | ATOM | 9574 | OG | SER B 225 | 22.795 | 55.133 | 20.625 | 1.00 51.40 | | • | С |
| | MOTA | 9576 | С | | | | 20.585 | 1.00 52.21 | | | ō |
| | MOTA | .9577 | 0 | SER B 225 | 23.838 | 55.743 | 21.159 | 1.00 32.21 | | | N |
| 25 | MOTA | 9578 | N | ILE B 226 | 21.681 | 55.609 | | | | | c |
| | ATOM | 9580 | CA | ILE B 226 | 21.652 | 56.966 | 21.677 | 1.00 47.18 | | • | . C. |
| | ATOM | 9582 | CB | ILE B 226 | 20.782 | 57.870 | 20.775 | 1.00 42.41 | | | |
| | ATOM | 9584 | CG1 | ILE B 226 | 19.421 | 57.276 | 20.563 | 1.00 36.20 | | | C |
| | MOTA | 9587 | | ILE B 226 | 18.355 | 58.275 | 20.220 | 1.00 36.28 | | | Ċ |
| 30 | MOTA | 9591 | CG2 | ILE B 226 | 21.425 | 58.015 | 19.433 | 1.00 45.19 | | | C |
| • • | MOTA | 9595 | С | ILE B 226 | 21.191 | 57.023 | 23.126 | 1.00 45.97 | | | С |
| | ATOM | 9596 | 0 | ILE B 226 | 20.610 | 56.051 | 23.598 | 1.00 43.09 | | | 0 |
| | ATOM | 9597 | N | VAL B 227 | 21.491 | 58.152 | 23.797 | 1.00 43.58 | . • | | N |
| | ATOM | 9599 | CA | VAL B 227 | 21.061 | 58.457 | 25.177 | 1.00 44.91 | | | С |
| 35 | ATOM | 9601 | CB | VAL B 227 | 22.211 | 59.070 | 26.001 | 1.00 40.77 | | | С |
| 33 | | 9603 | | VAL B 227 | 21.726 | | 27.313 | 1.00 40.80 | | | C |
| | MOTA | | | VAL B 227 | 23.360 | 58.096 | 26.187 | 1.00 38.82 | | • | C |
| | ATOM | 9607 | | VAL B 227 | 19.926 | 59.511 | 25.104 | 1.00 48.95 | | | С |
| | ATOM | 9611 | C | | | 60.617 | | 1.00 50.25 | | | Ō |
| 40 | ATOM | 9612 | 0 | VAL B 227 | 20.150 | | 25.624 | 1.00 44.84 | | | N |
| 40 | MOTA | 9613 | N | ASP B 228 | 18.730 | 59.205 | | | | | c |
| | MOTA | 9615 | CA | ASP B 228 | 17.565 | 60.043 | 25.336 | 1.00 40.47 | | | c |
| | MOTA | 9617 | CB | ASP B 228 | 16.936 | 59.514 | 24.036 | 1.00 38.92 | | | |
| | MOTA | 9620 | CG | ASP B 228 | 15.690 | 60.286 | 23.615 | 1.00 45.59 | | | С |
| | ATOM | 9621 | OD1 | ASP B 228 | 15.409 | 61.367 | 24.161 | 1.00 41.67 | | | 0 |
| 45 | MOTA | 9622 | OD2 | ASP B 228 | 14.903 | 59.871 | 22.744 | 1.00 55.53 | | | 0 |
| • | ATOM | 9623 | С | ASP B 228 | 16.512 | 60.133 | 26.470 | 1.00 43.36 | | | С |
| | MOTA | 9624 | 0 | ASP B 228 | 15.725 | 59.217 | 26.694 | 1.00 38.56 | | | 0 |
| | ATOM | 9625 | N. | SER B 229 | 16.488 | 61.267 | 27.164 | 1.00 47.36 | • | | N. |
| | ATOM | 9627 | CA | SER B 229 | 15.612 | 61.464 | 28.310 | 1.00 47.52 | | | C |
| 50 | ATOM | 9629 | CB | SER B 229 | 16.147 | 62.621 | 29.118 | 1.00 47.91 | | | C |
| 50 | | 9632 | OG · | SER B 229 | 16.818 | 63.473 | 28.231 | 1.00 51.18 | | | 0 |
| | ATOM | | | | 14.158 | 61.708 | 27.934 | 1.00 49.38 | | | C |
| | ATOM | 9634 | C | SER B 229 | | 61.994 | 28.798 | 1.00 54.96 | | | ō |
| | ATOM | 9635 | 0 | SER B 229 | 13.330 | | | | | | N |
| | MOTA | 9636 | N | GLY B 230 | | 61.632 | 26.644 | 1.00 48.92 | | | C |
| 55 | MOTA | 9638 | CA | GLY B 230 | 12.481 | 61.753 | 26.176 | 1.00 45.57 | | | |
| | MOTA | 9641 | С | GLY B 230 | 11.935 | 60.429 | 25.637 | 1.00 48.29 | | | C |
| | MOTA | 9642 | 0 | GLY B 230 | 10.833 | 60.372 | 25.085 | 1.00 40.94 | | | 0 |
| | ATOM | 9643 | N | THR B 231 | 12.735 | | 25.785 | 1.00 45.26 | | | N |
| | MOTA | 9645 | CA | THR B 231 | 12.303 | 58.035 | | | | | С |
| 60 | MOTA | 9647 | | THR B 231 | 13.349 | | 24.743 | 1.00 44.17 | | | C |
| 50 | ATOM | 9649 | | THR B 231 | 13.221 | | 23.350 | | | | 0 |
| | A1OI1 | 20,13 | 5.53 | | | | | · - | | | |

| 5 | ATOM | 9651 | CG2 | THR F | 3 231 | | 13.075 | 55.769 | 24.829 | 1.00 | 43.12 | | | С |
|------------|------|------|------|-------|----------------|---|--------|--------|--------|------|---------|---|-----|-----|
| , | ATOM | 9655 | C | | 3 231 | | 12.171 | 57.381 | 26.865 | 1.00 | 43.15 | | | С |
| | ATOM | 9656 | ō | | 3 231 | | 13.088 | 57.379 | 27.628 | 1.00 | 49.59 | | | 0 |
| | ATOM | 9657 | | | 3 232 | | 11.031 | 56.804 | 27.149 | | 45.08 | | | N |
| | | 9659 | CA | | 3 232 | | 10.801 | 56.103 | 28.393 | | 46.07 | | | С |
| 10 | MOTA | 9661 | СВ | | 3 232 | | 9.344 | 55.581 | 28.375 | | 43.69 | | | С |
| 10 | MOTA | | | | B 232 | | 8.475 | 56.653 | 27.964 | | 49.53 | | | 0 |
| | ATOM | 9663 | | | B 232 | | 8.867 | 55.276 | 29.748 | | 43.76 | | | C |
| | ATOM | 9665 | | | B 232 | | 11.759 | 54.905 | 28.630 | | 49.16 | | | С |
| | ATOM | 9669 | C | | B 232 | | 12.563 | 54.922 | 29.567 | | 51.59 | | | 0 |
| . ~ | ATOM | 9670 | | | | | 11.660 | 53.899 | 27.757 | | 51.81 | | | N |
| 15 | MOTA | 9671 | N | | B 233 | | 12.327 | 52.604 | 27.879 | | 50.18 | | - | ·C |
| | MOTA | 9673 | CA | | B 233 B 233 | | 11.655 | 51.566 | 26.967 | | 52.42 | | | C |
| | MOTA | 9675 | CB · | | | | | 51.148 | 27.383 | | 52.34 | | | Ċ |
| | ATOM | 9678 | CG | | B 233 | | 10.276 | | 28.321 | | 50.82 | | | ŏ |
| | MOTA | 9679 | | | B 233 | | 9.680 | 51.677 | 26.650 | | 52.61 | | | N. |
| 20 | MOTA | 9680 | | | В 233 | | 9.750 | 50.153 | | | 47.14 | | | C |
| | MOTA | 9683 | C | | B 233 | | 13.729 | 52.350 | 27.416 | | 46.63 | | | ō |
| | MOTA | 9684 | 0 | | В 233 | | 14.259 | 52.963 | 26.555 | | 47.70 | | | N |
| | ATOM | 9685 | N | | B 234 | | 14.306 | 51.355 | 28.019 | | | | | C |
| | MOTA | 9687 | CA | | B 234 | | 15.430 | 50.768 | 27.402 | | 51.03 | | | |
| 25 | MOTA | 9689 | CB | | В 234 | | 15.903 | 49.591 | 28.256 | | 47.48 | | | Ċ |
| | MOTA | 9692 | · CG | | B 234 | | 17.388 | 49.421 | 28.108 | | 44.91 | | | C |
| | ATOM | 9694 | | | B 234 | | 17.926 | 48.199 | 28.788 | | 47.69 | | | |
| | ATOM | 9698 | CD2 | | B 234 | | 17.643 | 49.365 | 26.676 | | 49.15 | | | C |
| | ATOM | 9702 | С | | B 234 | | 14.716 | 50.251 | 26.142 | | 53.66 | | | C |
| 30 | ATOM | 9703 | 0 | | B 234 | | 13.639 | 49.694 | 26.270 | | 57.67 | | | 0 |
| | MOTA | 9704 | N | | B 235 | | 15.262 | 50.431 | 24.945 | | 54.47 | | | N |
| | ATOM | 9706 | CA | ARG | B 235 | | 14.628 | 49.892 | 23.749 | | 50.55 | | - | C |
| | ATOM | 9708 | CB | | B 235 | | 14.146 | 50.948 | 22.782 | | 54.70 | | | . C |
| | MOTA | 9711 | CG | | B 235 | | 13.090 | 51.958 | 23.232 | | 60.77 | | | С |
| 35 | MOTA | 9714 | CD | ARG | B 235 | | 11.610 | 51.498 | 23.022 | | 63.38 | | | . C |
| • | ATOM | 9717 | NE | ARG | B 235 | , | 10.905 | 52.094 | 21.882 | | 65.81 | | | N |
| | ATOM | 9719 | CZ | ARG | B 235 | | 10.487 | 51.422 | 20.806 | | 68.02 | | | C |
| | ATOM | 9720 | NH1 | ARG | B 235 | | 9.854 | 52.062 | 19.844 | | 70.13 | | | N |
| | MOTA | 9723 | NH2 | ARG | B 235 | | 10.703 | 50.121 | 20.678 | | 68.31 | | | N |
| 40 | MOTA | 9726 | С | ARG | B 235 | | 15.799 | 49.326 | 23.069 | | 52.73 | | | С |
| | MOTA | 9727 | 0 | ARG | B 235 | | 16.794 | 50.033 | 22.960 | | 51.89 | | | 0 |
| | ATOM | 9728 | N | | B 236 | | 15.697 | 48.083 | 22.591 | | 53.67 | | | N |
| | ATOM | 9730 | CA | LEU | B 236 | | 16.816 | 47.414 | 21.951 | | 51.18 | | | С |
| | ATOM | 9732 | СВ | LEU | В 236 | | 17.336 | 46.273 | 22.857 | 1.00 | 54.12 | | | С |
| 45 | ATOM | 9735 | CG | LEU | B 236 | | 17.606 | 46.565 | 24.346 | 1.00 | 54.84 | | • | C |
| | ATOM | 9737 | CD1 | | B 236 | | 17.445 | 45.294 | 25,170 | 1.00 | 59.47 | | . ~ | C |
| | ATOM | 9741 | CD2 | LEU | В 236 | | 18.988 | | | 1.00 | 57.80 | | | С |
| | ATOM | 9745 | С | | B 236 | | 16.472 | 46.882 | 20.555 | 1.00 | 49.66 | | | С |
| | ATOM | 9746 | ō | | B 236 | | 15.320 | 46.574 | 20.244 | 1.00 | 51.23 | | | 0 |
| 50 | ATOM | 9747 | N | | В 237 | | 17.516 | 46.802 | 19.740 | | 49.55 | | | N |
| . 50 | ATOM | 9748 | CA | | B 237 | | 17.528 | 46.266 | 18.364 | | 53.89 | | | C |
| | ATOM | 9750 | CB | | B 237 | | 19.037 | 46.236 | 18.036 | | 52.34 | | | С |
| | | 9753 | CG | | B 237 | | 19.634 | 47.291 | 18.888 | | 51.34 | | | С |
| | ATOM | | CD | | B 237 | | 18.837 | 47.302 | 20.146 | | 49.53 | • | | С |
| 55 | ATOM | 9756 | C | | B 237 | | 17.003 | 44.846 | 18.178 | | 55.60 | | : | C |
| 55 | ATOM | 9759 | 0 | | B 237 | | 17.524 | 43.944 | 18.794 | | 51.46 | | | Ō |
| | ATOM | 9760 | | | B 238 | • | | 44.660 | 17.297 | | 62.69 | | | N |
| | MOTA | 9761 | N | | | | 16.027 | 44.000 | 17.149 | | 62.37 | | | c |
| | MOTA | 9763 | CA | | B 238 | | 15.321 | 43.380 | | | 63.90 | | | c |
| ~ ^ | ATOM | 9765 | CB | | B 238 | | 14.847 | | 15.476 | | 0 67.48 | | | č |
| 60 | MOTA | 9768 | CG | | B 238 | | 14.017 | 41.850 | | | 70.44 | | | č |
| | ATOM | 9771 | CD | ГЛЭ | B 238 | | 12.652 | 41.826 | 10.191 | 1.00 | J /U.44 | | | _ |

| 5 | ATOM | 9774 | CE | LYS | B 238 | 1 | 2.375 | 40.445 | 16.872 | 1.00 | 75.03 | • | С |
|---------|-----------|-------|------------|-----|-------|---|------------------|--------|--------|------|-------|---|--------|
| | ATOM | 9777. | NZ | | B 238 | | 0.906 | 40.068 | 17.069 | | 74.40 | | N |
| | ATOM | 9781 | С | LYS | B 238 | 1 | 6.015 | 42.134 | 17.728 | 1.00 | 60.78 | | С |
| | ATOM | 9782 | 0 | LYS | B 238 | | 5.417 | 41.472 | 18.563 | 1.00 | 63.50 | | 0 |
| | ATOM | 9783 | N | | B 239 | 1 | 7.242 | 41.808 | 17.318 | 1.00 | 62.12 | | N |
| 10 | ATOM | 9785 | CA | | В 239 | | 7.976 | 40.613 | 17.832 | 1.00 | 62.88 | | С |
| •• | ATOM | 9787 | СВ | | B 239 | | 9.245 | 40.375 | 17.004 | | 63.86 | | C |
| • | ATOM | 9790 | CG | | B 239 | | 9.081 | 39.310 | 15.932 | | 71.17 | | С |
| | ATOM | 9793 | CD | | B 239 | | 0.316 | 39.144 | 15.035 | 1.00 | 73.03 | | С |
| • | ATOM | 9796 | CE | | B 239 | | 0.418 | 37.713 | 14.440 | | 74.08 | | С |
| 15 | ATOM | 9799 | NZ | | B 239 | | 0.797 | 37.688 | 12.972 | | 69.81 | | N |
| 1.5 | ATOM | 9803 | C | | B 239 | | 8.422 | 40.587 | 19.317 | 1.00 | 63.28 | | С |
| | ATOM | 9804 | ō | | B 239 | | 8.587 | 39.508 | 19.896 | | 62.95 | | 0 |
| | ATOM | 9805 | N T | | B 240 | | 8.627 | 41.760 | 19.915 | | 58.01 | | N |
| | ATOM | 9807 | CA | | B 240 | | 9.131 | | 21.269 | | 54.79 | | C |
| 20 | ATOM | 9809 | CB | | B 240 | | 9.827 | 43.225 | 21.427 | | 58.03 | | C |
| 20 | ATOM | 9811 | | | B 240 | | 0.256 | 43.484 | 22.875 | | 57.45 | | C |
| | ATOM | 9815 | | | B 240 | | 1.047 | 43.292 | 20.450 | | 57.36 | | C |
| | ATOM | 9819 | C | | B 240 | | 7.964 | 41.707 | 22.220 | | 56.00 | | Č |
| | ATOM | 9820 | | | B 240 | | 7.980 | 40.890 | 23.143 | | 52.22 | | ō |
| 25 | ATOM | 9821 | N | | B 241 | | 6.928 | 42.488 | 22.012 | | 55.23 | • | N |
| 23 | ATOM | 9823 | CA | | B 241 | | 5.725 | 42.212 | 22.742 | | 53.80 | | C |
| | ATOM | 9825 | CB | | B 241 | | 4.545 | 42.796 | 22.032 | | 51.30 | | Č |
| | ATOM | 9828 | CG | | B 241 | | 3.300 | 42.770 | 22.822 | | 47.65 | | Č |
| | ATOM | 9829 | | | B 241 | | 3.154 | 43.590 | 23.937 | | 48.68 | | č |
| 30 | ATOM | 9831 | | | B 241 | | 1.997 | 43.588 | 24.677 | | 50.08 | | c |
| 30 | ATOM ATOM | 9833 | CZ | | B 241 | | .0.952 | 42.755 | 24.315 | | 51.83 | | č |
| | ATOM | 9835 | | | B 241 | | 1.085 | 41.930 | 23.193 | | 54.34 | | Č |
| | ATOM | 9837 | | | B 241 | | 2.267 | 41.953 | 22.451 | | 52.82 | | Č |
| | ATOM | 9839 | CDZ | | B 241 | | 5.546 | 40.714 | 22.793 | | 55.05 | | c |
| 35 | ATOM | 9840 | o | | B 241 | | 5.660 | 40.714 | 23.852 | | 58.72 | | ő |
| <i></i> | ATOM | 9841 | N | | B 242 | | 15.296 | 40.080 | 21.651 | | 58.90 | | N |
| | ATOM | 9843 | CA | | B 242 | | 4.915 | 38.650 | 21.665 | | 61.77 | | c |
| | ATOM | 9845 | CB | | B 242 | | 4.771 | 38.033 | 20.255 | | 64.23 | | c |
| | ATOM | 9848 | CG | | B 242 | | 13.434 | 38.214 | 19.518 | | 66.72 | | Č |
| 40 | ATOM | 9851 | CD | | B 242 | | 12.187 | 37.837 | 20.319 | | 73.25 | | Č |
| 70 | ATOM . | 9852 | | | B 242 | | 11.766 | | 20.267 | | 74.25 | | ō |
| | ATOM | 9853 | | | B 242 | | 11.605 | | 20.207 | | 80.65 | | ŏ |
| | ATOM | 9854 | C | | B 242 | | 15.946 | | 22.473 | | 60.51 | | Č |
| | ATOM | 9855 | Ö | | B 242 | | 15.606 | | 23.317 | | 61.16 | | ŏ |
| 45 | ATOM | 9856 | N | | B 243 | | 17.221 | 38.094 | 22.222 | | 59.55 | | N |
| 73 | ATOM | 9858 | CA | | B 243 | | 18.246 | | 22.981 | | 54.76 | | C |
| | ATOM | 9860 | | | B 243 | | 19.628 | 37.910 | 22.546 | | 50.14 | | ď |
| | | | | | B 243 | | 18.056 | | | | 57.05 | | Č |
| | MOTA | 9864 | C | | | | 18.157 | | 25.272 | | 60.16 | | ő |
| 50 | ATOM | 9865 | 0 | | B 243 | | | | 24.872 | | 60.67 | | N |
| 30 | ATOM | 9866 | N | | B 244 | | 17.764 17.847 | | 26.277 | | 56.99 | | C |
| | ATOM | 9868 | CA | | B 244 | | | | 26.396 | | 54.73 | | C |
| | MOTA | 9870 | CB | | B 244 | | 17.983 16.670 | | | | | | C |
| | ATOM | 9874 | C . | | B 244 | | | | 27.039 | | 57.52 | | |
| | MOTA | 9875 | 0 | | B 244 | | 16.814 | | 28.022 | | 66.61 | | 0 |
| 55 | ATOM | 9876 | . N | | B 245 | | 15.497 | | 26.578 | | 58.39 | | N C |
| • | MOTA | 9878 | CA | | B 245 | | 14.264 | | 27.182 | | 57.61 | | |
| | ATOM | 9880 | CB | | B 245 | | 13.084 | | 26.272 | | 55.77 | | C |
| | ATOM | 9882 | | | B 245 | | 11.921 | | 26.582 | | 60.16 | | С |
| ćo | ATOM | 9886 | | | B 245 | | 12.682 | | 26.425 | | 55.68 | | C |
| 60 | ATOM | 9890 | С | | B 245 | | 14.276 | | 27.445 | | 56.76 | | C |
| | MOTA | 9891 | 0 | VAL | B 245 | | 13.735 | 36.630 | 28.457 | 1.00 | 58.98 | | 0 |
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14.863
                                               36.289
                                                       26.581
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                  CA
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                       LYS B 246
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                       ILE B 248
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                   С
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60
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                                       11.876
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                                                        41.285
                                                                 1.00 55.22
            10012
                        THR B 254
     MOTA
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|-------------|------|-------|-------|-------|-------|---|--------|--------|---------|------|---------|---|----|----|
| 5 | MOTA | 10014 | OG1 ' | | | | 12.383 | 32.851 | 41.131 | | 59.23 | | | 0 |
| | MOTA | 10016 | CG2 ' | THR E | 3 254 | | 13.081 | 30.702 | 41.690 | | 57.98 | • | | C |
| | ATOM | 10020 | C ' | THR E | 3 254 | | 9.853 | 31.304 | 39.850 | | 56.31 | | | Ċ |
| | ATOM | 10021 | 0 ' | THR E | 3 254 | | 9.067 | 30.740 | 40.587 | | 58.63 | • | | 0 |
| | ATOM | 10022 | N (| GLU E | 3 255 | | 9.496 | 32.222 | 38.954 | | 63.22 | | | N |
| 10 | ATOM | 10024 | | GLU I | 3 255 | | 8.081 | 32.520 | 38.661 | | 64.71 | | | С |
| 10 | ATOM | 10026 | | | 3 255 | | 7.691 | 33.884 | 39.210 | | 64.18 | | | С |
| | ATOM | 10029 | | | 3 255 | | 7.814 | 33.921 | 40.721 | 1.00 | 65.62 | | | С |
| | ATOM | 10032 | | | 3 255 | | 6.988 | 35.013 | 41.364 | | 65.81 | | | C |
| | | 10032 | | | 3 255 | | 5.941 | 35.412 | 40.801 | 1.00 | 65.88 | | | 0 |
| 15 | ATOM | 10033 | | | B 255 | | 7.398 | 35.458 | 42.452 | 1.00 | 67.44 | | | 0 |
| 15 | ATOM | 10034 | | | B 255 | | 7.843 | 32.474 | 37.155 | 1.00 | 65.92 | | | С |
| | MOTA | 10035 | | | B 255 | | 8.761 | 32.231 | 36.374 | | 67.96 | | | 0 |
| | ATOM | | | | B 256 | | 6.611 | 32.686 | 36.737 | | 64.15 | | | N |
| | | 10037 | | | | | 6.347 | 32.771 | 35.319 | | 62.25 | | | С |
| | MOTA | 10039 | | | B 256 | | 5.753 | 31.487 | 34.780 | | 65.89 | | | С |
| 20 | MOTA | 10041 | | | B 256 | | 6.795 | | 34.631 | | 70.21 | | | С |
| | MOTA | 10044 | | | B 256 | | | 30.472 | 33.304 | | 71.31 | | | С |
| | MOTA | 10047 | | | B 256 | | 7.580 | | 33.197 | | 70.80 | | | c |
| | ATOM | 10050 | | | В 256 | | 8.688 | 29.418 | 34.535 | | 71.41 | | | N |
| | MOTA | 10053 | | | В 256 | | 9.037 | 28.832 | | | 61.03 | | | c |
| 25 | MOTA | 10057 | | | B 256 | | 5.414 | 33.918 | 35.091 | | 57.24 | | | ŏ |
| • | ATOM | 10058 | 0 | | В 256 | | 4.620 | 34.277 | 35.977 | | | | | N |
| | MOTA | 10059 | N | | B 257 | | 5.522 | 34.500 | 33.903 | | 57.37 | | | C |
| | ATOM | 10061 | CA | | В 257 | | 4.700 | 35.632 | 33.563 | | 58.14 | | | c |
| | ATOM | 10063 | CB | PHE | В 257 | | 5.557 | 36.904 | 33.635 | | 57.69 | | | |
| 30 | MOTA | 10066 | CG | | В 257 | | 6.262 | 37.095 | 34.971 | | 52.26 | | | C |
| | MOTA | 10067 | | | В 257 | | 7.620 | 36.875 | 35.098 | | 55.74 | | | C |
| | ATOM | 10069 | CE1 | PHE | B 257 | | 8.248 | 37.044 | 36.298 | | 55.86 | | | C |
| | MOTA | 10071 | CZ | PHE | B 257 | | 7.530 | 37.444 | 37.391 | | 56.14 | | | С |
| | ATOM | 10073 | CE2 | PHE | B 257 | | 6.194 | 37.666 | 37.274 | | 54.82 | | | C. |
| 35 . | ATOM | 10075 | CD2 | PHE | B 257 | | 5.569 | 37.490 | 36.073 | | 49.91 | | | C |
| | ATOM | 10077 | С | PHE | В 257 | | 4.089 | 35.397 | 32.177 | | 61.13 | | | C |
| | ATOM | | . 0 | PHE | В 257 | | 4.687 | 34.705 | 31.356 | | 60.35 | | | 0 |
| | ATOM | 10079 | N | | B 258 | | 2.902 | 35.964 | 31.934 | | 64.44 | | | N |
| | ATOM | 10080 | CA | | B 258 | | 2.175 | 35.834 | 30.651 | 1.00 | 67.15 | | | С |
| 40 | ATOM | 10082 | CB | | В 258 | | 0.765 | 36.286 | 31.018 | | 65.96 | | | С |
| 10 | ATOM | 10085 | CG | | B 258 | | 0.946 | 37.246 | .32.161 | | 63.58 | | | С |
| | ATOM | 10088 | CD | | B 258 | | 2.172 | 36.804 | 32.906 | 1.00 | 63.13 | | | C |
| | ATOM | 10091 | C | | B 258 | | 2.740 | 36.758 | 29.561 | 1.00 | 71.79 | | | С |
| | ATOM | 10092 | ŏ | | B 258 | | 2.885 | | 29.830 | 1.00 | 76.81 | | | 0 |
| 45 | ATOM | 10093 | N | | B 259 | | 3.010 | 36.250 | 28.357 | 1.00 | 73.38 | | | N |
| 43 | ATOM | 10095 | CA | | B 259 | • | 3.820 | 36.980 | 27.356 | 1.00 | 75.86 | | | С |
| · .• | ATOM | 10097 | CB | | B 259 | | 3.890 | 36.221 | 26.029 | 1.00 | 77.62 | | | С |
| | | | CG | | B 259 | | 3.803 | | 26.222 | 1.00 | 78.97 | | ٠. | С |
| | MOTA | | | | B 259 | | 4.731 | 33.953 | 25.816 | | 0 64.34 | | | 0 |
| ·50 | ATOM | 10101 | | | B 259 | | | | 26.786 | | 80.20 | | | 0 |
| 50 | ATOM | 10102 | | | B 259 | | 3.443 | | 27.102 | | 0 76.48 | | | С |
| | MOTA | | С | | | | 4.216 | | | | 0 74.95 | | | 0 |
| | ATOM | 10104 | 0 | | B 259 | | 2.259 | | | | 0 75.19 | | | N |
| | ATOM | | N | | B 260 | • | | | | | 0 72.78 | | | С |
| | MOTA | | CA | | B 260 | | 1.905 | | | | 0 68.86 | | | Ċ |
| 55 | ATOM | | С | | B 260 | | 2.926 | | | | 0.70.54 | | | ō |
| | ATOM | | 0 | | B 260 | | 3.429 | | | | | | | N |
| | ATOM | | N | | B 261 | | 3.239 | | | | 0 65.94 | • | | C |
| • | ATOM | | CA | | B 261 | | 4.187 | | | | 0 61.43 | | | c |
| | MOTA | | | | B 261 | | 4.317 | | | | 0 56.82 | | | c |
| 60 | ATOM | 10119 | | | B 261 | | 5.391 | | | | 0 54.73 | | | Ç |
| | ATOM | 10120 | CD1 | PHE | B 261 | | 5.126 | 41.944 | 33.382 | 1.0 | 0 51.57 | | | C |
| | | | | | | | | | | | | | | |

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1.00 51.52
                                                                                   · C
                                                       34.188
                  CE1 PHE B 261
                                       6.106
                                               42.488
    MOTA
          10122
                                                                1.00 57.72
                                                       34.166
                  CZ PHE B 261
                                               41.961
                                       7.365
    MOTA
          10124
                                                                1.00 57.74
                  CE2 PHE B 261
                                       7.658
                                               40.876
                                                       33.345
          10126
    MOTA
                                                                1.00 59.54
                                                       32.550
                  CD2 PHE B 261
                                       6.676
                                               40.343
    ATOM
          10128
                                                       29.876
                                                                1.00 57.86
                                               41.195
                       PHE B 261
                                       5.603
    MOTA
           10130
                  С
                                                       30.377
                                                                1.00 68.09
                                       6.386
                                               41.981
                       PHE B 261
10
    MOTA
          .10131
                  0
                                                                                      N
                                                       28.892
                                                                1.00 56.00
                                       5.954
                                               40.389
     ATOM
           10132
                  N
                       TRP B 262
                                                                                      С
                                                                1.00 56.28
                                                       28.263
                                       7.253
                                               40.518
                       TRP B 262
     MOTA
           10134
                  CA
                                                                                      C
                                                                1.00 54.41
                                               39.170
                                                       28.049
                       TRP B 262
                                       7.932
     MOTA
           10136
                  CB
                                                               1.00 55.03
                                                                                      С
                                               38.278
                                                       29.238
                                       8.136
                       TRP B 262
                  CG
     MOTA
           10139
                                                                1.00 52.81
                                                       29.525
                                                                                      C
                  CD1 TRP B 262
                                       7.407
                                               37.184
15
           10140
     MOTA
                                                                1.00 58.02
                                                       30.669
                                       7.866
                                               36.578
           10142
                  NE1 TRP B 262
     MOTA
                                                       31.156
                                                                1.00 56.77
                   CE2 TRP B 262
                                       8.931
                                               37.281
           10144
     ATOM
                                                                1.00 63.26
                                                                                      C
                                               38.379
                                                       30.276
                   CD2 TRP B 262
                                       9.135
    MOTA
           10145
                                                                1.00 54.90
                                                        30.552
                                               39.274
                   CE3 TRP B 262
                                      10.180
     MOTA
           10146
                                                                1.00 55.79
                                                        31.685
                                      10.970
                                               39.046
20
           10148
                   C23 TRP B 262
     MOTA
                                                                1.00 54.57
                                               37.955
                                                        32.537
                                      10.733
                   CH2 TRP B 262
     MOTA
           10150
                                                                1.00 53.00
                                                        32.288
                   CZ2 TRP B 262
                                       9.717
                                               37.063
           10152
     MOTA
                                                                1.00 55.99
                                                        26.932
                                       7.104
                                               41.282
           10154
                   С
                       TRP B 262
     MOTA
                                                                1.00 59.38
                                                        26.231
                       TRP B 262
                                       8.062
                                               41.510
           10155
                   0
     MOTA
                                                                1.00 57.34
                                                        26.565
                                               41.686
25
           10156
                   N
                       LEU B 263
                                       5.907
     ATOM
                                                                1.00 55.32
                                                       25.461
                                       5.811
                                               42.625
           10158
                   CA
                       LEU B 263
     ATOM
                                                                                      С
                                                                1.00 55.06
                                               42.116
                                                        24.311
           10160
                   CB
                       LEU B 263
                                        4.939
     ATOM
                                                                                      С
                                                        23.756
                                                                1.00 50.87
                                        5.272
                                               40.716
                       LEU B 263
     MOTA
           10163
                   CG
                                                                1.00 53.49
                                                                                      C
                   CD1 LEU B 263
                                       4.008
                                               40:071
                                                        23.221
     MOTA
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                                                                                      C
                                        6.315
                                                        22.680
                                                                1.00 50.09
                   CD2 LEU B 263
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30
     MOTA
                                                                1.00 57.11
                                                                                     . C
                                                        26.099
                       LEU B 263
                                        5.282
                                               43.907
           10173
     MOTA
                   С
                                                        25.449
                                                                                      0
                                                               1.00 62.05
                                        4.669
                                               44.749
           10174
                   0
                       LEU B 263
     MOTA
                                                                1.00 58.91
                                                                                      N
                                               44.039
                                                        27.400
                       GLY B 264
                                       5.520
           10175
     MOTA
                                                                                      C
                                       5.227
                                                        28.129
                                                                1.00 59.68
                                               45.268
                       GLY B 264
     MOTA
           10177
                   CA
                                        3.855
                                                45.865
                                                        27.896
                                                                1.00 59.63
                                                                                      С
                       GLY B 264
                   С
35
           10180
     ATOM
                                                                1.00 64.20
                                                                                      0
                                                        28.142
                       GLY B 264
                                      3.643
                                                47.054
           10181
                   0
     MOTA
                                                                1.00 60.98
                                                                                      N
                                                        27.441
           10182
                       GLU B 265
                                        2.918
                                                45.042
     MOTA
                   N
                                                                1.00 64.98
                                                        27.189
                                                                                       С
                                                45.480
                                        1.547
     ATOM
           10184
                   CA
                       GLU B 265
                                                                                       С
                                                                1.00 66.91
                                        0.878
                                                44.484
                                                        26.249
                       GLU B 265
     MOTA
            10186
                   CB
                                                                                       С
                                                                1.00 74.60
                                                        24.795
                                        0.967
                                                44.902
40
                       GLU B 265
     MOTA
           10189
                   CG
                                                                1.00 81.19
                                                                                      ·C
                                        0.904
                                                43.720
                                                        23.835
                       GLU B 265
     MOTA
            10192
                   CD
                                                                1.00 80.62
                                                                                       0
                                        1.023
                                                43.968
                                                        22.603
            10193
                   OE1 GLU B 265
     MOTA
                                                                1.00 85.40
                                                42.556
                                                        24.311
            10194
                   OE2
                       GLU B 265
                                        0.734
     MOTA
                                                                1.00 66.06
                                                45.595
                                                        28.433
                                        0.674
            10195
                       GLU B 265
     MOTA
                   С
                                       -0.178
                                                46.471
                                                        28.534
                                                                1.00 67.79
                       GLU B 265
45
     ATOM
            10196
                   0
                                        0.890
                                                       29.368
                                                                1.00 65.41
                       GLN B 266
                                                44.677
            10197
     MOTA
                   N
                                                                                       С
                                                                1.00 66.17
                                        0.029
                                                44.521
                                                        30.539
                       GLN B 266
            10199
                   CA
     MOTA
                                                                1.00 66.49
                                       -0.860
                                                43.299
                                                        30.402
            10201
                   CB
                       GLN B 266
     MOTA
                                                                1.00 66.76
                                       -0.090
                                                42.024
                                                        30.448
            10204
                   ·CG
                       GLN B 266
     MOTA
                                                                1.00 71.05
                                                        30.044
50
     MOTA
            10207
                   CD
                       GLN B 266
                                       -0.932
                                                40.851
                                                                1.00 78.94
                                                                                       0
                                       -0.926
                                                40.453
                                                        28.881
     ATOM
            10208
                   OE1 GLN B 266
                                                                                       N
                                       -1.660
                                                40.282
                                                        30.996
                                                                1.00 65.67
                   NE2 GLN B 266
     MOTA
            10209
                                                                                       С
                                                                 1.00 66.63
                                        0.880
                                                44.359
                                                        31.773
            10212
                        GLN B 266
     MOTA
                   С
                                                                                       0
                                        1.998
                                                        31.714
                                                                 1.00 61.37
                        GLN B 266
                                                43.881
            10213
     ATOM
                   0
                                                        32.910 1.00 68.01
                                                                                       N
                                        0.335
                                                44.745
            10214
                        LEU B 267
55
     MOTA
                   N
                                                                                       С
                       LEU B 267
                                        1.196
                                                44.910
                                                        34.055
                                                                 1.00 66.65
            10216
                   CA
      MOTA
                                                        34.780
                                                                 1.00 64.75
      MOTA
            10218
                   CB
                        LEU B 267
                                        0.782
                                                46.202
                                                                 1.00 61.97
                                       -0.664
                                                46.456
                                                        35.117
      MOTA
            10221
                   CG
                        LEU B 267
                                       -0.953
                                                45.596
                                                        36.275
                                                                 1.00 65.54
                   CD1 LEU B 267
      MOTA
            10223
                                       -0.883
                                                        35.487
                                                                 1.00 62.67
                   CD2 LEU B 267
                                                47.886
   MOTA
            10227
                                        1.305
                                                43.674
                                                        34.947
                                                                 1.00 66.02
                        LEU B 267
      MOTA
            10231 C
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| | | | | | | | | | | | • | | | | | |
|------|--------|-------|-----|------------|------|-----------|-----|----|-------|--------|--------|------|---------|---|---|-----|
| 5 | ATOM | 10232 | o | LEU I | 3 26 | 57 | | | 0.742 | 42.633 | 34.643 | | 65.04 | | | О |
| | MOTA | 10233 | N | VAL 1 | B 26 | 58 | | : | 2.062 | 43.779 | 36.031 | | 66.18 | | | N |
| | ATOM | 10235 | CA | VAL | B 26 | . 85 | | : | 2.201 | 42.665 | 36.966 | | 63.11 | | | С |
| | ATOM | 10237 | CB | VAL | B 26 | 58 | | | 3.526 | 42.035 | 36.844 | | 63.47 | | | С |
| | ATOM | 10239 | CG1 | VAL 1 | B 26 | 8 | | | 3.584 | 40.817 | 37.674 | | 65.01 | | | C. |
| 10 | ATOM | 10243 | CG2 | VAL | B 26 | 8 | | | 3.741 | 41.689 | 35.434 | | 67.71 | | | ·C |
| | ATOM | 10247 | С | VAL | B 20 | 58 | | | 2.089 | 43.146 | 38.376 | 1.00 | 62.57 | | | С |
| | ATOM | 10248 | 0 | VAL | B 20 | 58 | | | 2.535 | 44.227 | 38.723 | 1.00 | 64.30 | | | 0 |
| | ATOM | 10249 | N | CYS | B 2 | 59 | | | 1.498 | 42.320 | 39.204 | | 62.51 | | | N |
| | ATOM | 10251 | CA | CYS | B 2 | 69 | | | 1.189 | 42.742 | 40.543 | 1.00 | 62.84 | | | С |
| 15 | ATOM | 10253 | CB | CYS | | | | _ | 0.334 | 42.937 | 40.667 | 1.00 | 64.89 | | | С |
| 10 | ATOM | 10256 | SG | CYS | | | | _ | 0.978 | 44.253 | 39.612 | 1.00 | 68.14 | | | S |
| | ATOM | 10257 | С | CYS : | | | | | 1.677 | 41.778 | 41.610 | 1.00 | 58.60 | | | С |
| | ATOM | 10258 | 0 | CYS | | | | | 1.707 | 40.556 | 41.420 | 1.00 | 57.72 | | | 0 |
| • | ATOM | 10259 | N | TRP | | | • | | 2.040 | 42.374 | 42.731 | 1.00 | 50.46 | | | N |
| 20 | ATOM | 10261 | CA | TRP | | | . ' | | 2.483 | 41.669 | 43.896 | 1.00 | 53.90 - | | | C |
| 20 | ATOM | 10263 | СВ | TRP | | | | | 3.996 | 41.833 | 44.087 | 1.00 | 54.89 | | | С |
| | ATOM | 10266 | CG | TRP | | | | | 4.740 | 40.871 | 43.267 | 1.00 | 55.99 | | | С |
| | ATOM | 10267 | CD1 | TRP | | | | | 4.829 | 39.543 | 43.480 | 1.00 | 57.11 | | | C. |
| | MOTA | 10269 | NE1 | | | | | | 5.601 | 38.961 | 42.503 | 1.00 | 61.98 | | | N |
| 25 | ATOM | 10271 | | TRP | | | | | 6.026 | 39.929 | 41.633 | | 61.92 | | | С |
| 23 | ATOM | 10272 | | TRP | | | | | 5.500 | 41.145 | 42.081 | | 57.92 | | | С |
| | ATOM | 10273 | | TRP | | | | | 5.793 | 42.297 | 41.355 | | 53.37 | | | С |
| | ATOM | 10275 | | TRP | | | | | 6.571 | 42.199 | 40.241 | 1.00 | 53.54 | | | С |
| | ATOM | 10277 | | TRP | | | | | 7.083 | 40.982 | 39.812 | | 56.68 | | | С |
| 30 - | ATOM | 10279 | | TRP | | | | | 6.825 | 39.834 | 40.490 | 1.00 | 64.93 | | | C |
| 50 | ATOM | 10281 | C | TRP | | | | | 1.753 | 42.293 | 45.048 | | 52.99 | | | Ç |
| | ATOM | 10282 | Ö | TRP | | | | | 1.321 | 43.432 | 44.976 | | 52.30 | | | 0 |
| | MOTA | 10283 | N | GĻN | | | | | 1.612 | 41.554 | 46.126 | | 56.53 | | | N |
| | ATOM | 10285 | CA | GLN | | | | | 0.897 | 42.083 | 47.267 | | 58.01 | | | С |
| 35 | ATOM - | 10203 | CB | GLN | | | | | 0.936 | 41.079 | 48.415 | | 60.04 | | | С |
| 33 | MOTA | 10290 | CG | GLN. | | | | | 0.773 | 41.648 | 49.826 | | 69.55 | | | С |
| | ATOM | 10293 | CD | GLN | | | | | 1.280 | 40.664 | 50.910 | | 75.84 | | | С |
| | ATOM | 10294 | | GLN | | | | | 2.450 | 40.268 | 50.900 | | 78.40 | | | 0 |
| | ATOM | 10295 | | GLN | | | | | 0.392 | 40.262 | 51.825 | | 80.06 | | • | N |
| 40 | ATOM | 10298 | C | GLN | | | | | 1.683 | | 47.553 | | 54.15 | | | С |
| •• | ATOM | 10299 | Ö | GLN | | | | | 2.781 | 43.454 | 47.050 | | 62.98 | | • | 0 |
| | ATOM | 10300 | N | ALA | | | | | 1.162 | 44.209 | 48.341 | 1.00 | 54.28 | | | N |
| | ATOM | 10302 | CA | ALA | | | | | 1.964 | 45.351 | 48.683 | 1.00 | 55.76 | | | С |
| | ATOM | 10304 | CB | ALA | | | | | 1.280 | 46.192 | 49.767 | 1.00 | 54.56 | | | С |
| 45 | ATOM | 10308 | | ALA | | | | | 3.325 | 44.876 | 49.169 | | 57.86 | | | С |
| .5 | ATOM | 10309 | ŏ | ALA | | | | | 3.497 | 43.739 | 49.579 | | 57.62 | | | 0 |
| | ATOM | 10310 | N | GLY | | | | • | 4.296 | 45.776 | 49.067 | 1.00 | 64.15 | | | N |
| | ATOM | 10312 | CA | GLY | | | | | | 45.660 | 49.699 | 1.00 | 62.02 | | | С |
| | ATOM | 10315 | C | GLY | | | | | 6.435 | 44.431 | 49.502 | | | | | С |
| 50 | ATOM | 10316 | ō | GLY | | | | | 7.544 | 44.376 | 50.003 | | 62.91 | | | 0 |
| ,50 | ATOM | 10317 | N | THR | | | | | 5.926 | 43.467 | 48.751 | | 59.03 | | | N |
| | ATOM | 10319 | CA | THR | | | | | 6.529 | 42.155 | 48.713 | | 52.35 | | | С |
| | ATOM | 10321 | СВ | THR | | | | | 5.483 | 41.091 | 49.087 | | 58.59 | | | С |
| | ATOM | 10323 | | THR | | | | | 4.574 | 40.872 | 47.988 | | 54.95 | | | . 0 |
| 55 | ATOM | 10325 | | THR | | | | | 4.593 | 41.579 | 50.243 | | 55.11 | | | C |
| | ATOM | 10329 | C. | THR | | | | | 6.971 | 41.857 | 47.351 | | 46.12 | | | Ċ. |
| | | 10329 | o | THR | | | | ٠. | 6.961 | 40.726 | 46.957 | | 46.68 | | | ō |
| | ATOM. | 10330 | N | | | | • | ٠. | 7.332 | 42.868 | 46.600 | | 47.81 | | | N |
| | ATOM | 10333 | CA | THR THR | | | | | 7.866 | | | | 48.64 | | | C |
| 60 | ATOM | | | | | | | | 8.257 | 43.907 | 44.540 | | 47.68 | | | č |
| 60 | ATOM | 10335 | CB | THR | | | | | 7.090 | | 44.064 | | 50.08 | | | ő |
| | MOTA | 10337 | OGI | THR | B 2 | 275 | | | 7.050 | | 27.004 | 1.00 | . 50.00 | • | | J |

| | | | | | | | 0.005 | 42 551 | 43.276 | 1 00 | 46.87 | | | 1 | С |
|-----|--------|-------|------|--------|---------|---|--------|---------|---------|-------|---------|---|----|---|------|
| 5 | | | CG2 | | В 275 | | 9.005 | 43.551 | 45.539 | 1 00 | 51.15 | | | | С |
| | MOTA | 10343 | С | | в 275 | | 9.114 | 41.783 | | | 54.79 | | • | | 0 |
| | ATOM | 10344 | 0 | | В 275 | | 9.984 | 42.143 | 46.371 | | 46.67 | | | | N |
| | ATOM | 10345 | N | | B 276 | | 9.190 | 40.685 | 44.822 | | | | | | c · |
| | ATOM | 10346 | CA | PRO | B 276 | | 10.355 | 39.808 | 44.811 | | 48.43 | | _ | | C |
| 10 | ATOM | 10348 | CB | PRO | B 276 | | 9.895 | 38.611 | 43.955 | | 50.23 | | - | | |
| 10 | ATOM | 10351 | CG | | В 276 | | 8.574 | 38.955 | 43.383 | | 51.47 | | | | С |
| | | 10354 | CD | | B 276 | | 8.101 | 40.227 | 43.956 | 1.00 | 50.10 | | | | С |
| | MOTA | | | | B 276 | | 11.557 | 40.420 | 44.091 | 1.00 | 48.73 | | | | С |
| | MOTA | 10357 | С | | B 276 | | 12.010 | 39.796 | 43.088 | 1.00 | 44.55 | | | | 0 |
| | ATOM | 10358 | 0. | | | | 12.013 | 41.567 | 44.537 | 1.00 | 48.39 | | | | N |
| 15 | MOTA | 10359 | | TRP | В 277 | | | 42.230 | 43.711 | | 48.55 | • | | | С |
| | MOTA | 10361 | CA | | B 277 | | 13.120 | 43.469 | 44.393 | | 48.09 | | | | C. |
| | ATOM | 10363 | CB | | В 277 | | 13.740 | | | | 50.79 | | | | С |
| | ATOM | 10366 | CG | | B 277 | | 12.769 | 44.677 | 44.518 | | 54.20 | | | | č |
| • | ATOM | 10367 | CD1 | TRP | В 277 | | 12.309 | 45.236 | 45.680 | | | | | | N |
| 20 | MOTA | 10369 | NE1 | TRP | B 277 | | 11.463 | 46.285 | | | 46.92 | | | | C |
| 20 | ATOM | 10371 | CE2 | TRP | В 277 | | 11.359 | 46.429 | 44.063 | | 42.74 | | | | |
| | ATOM | 10372 | CD2 | TRP | B 277 | | 12.164 | 45.439 | 43.466 | | 47.17 | | | | C |
| | MOTA | 10372 | | | В 277 | | 12.222 | 45.390 | 42.078 | | 51.68 | | | | C |
| | | | C73 | TRP | B 277 | | 11.486 | 46.318 | 41.352 | | 46.11 | | | | С |
| 0.5 | MOTA | 10375 | 0112 | UDD D | В 277 | | 10.703 | 47.270 | 41.991 | 1.00 | 45.63 | | | | С |
| 25 | ATOM | 10377 | | TIVE | В 277 | | 10.626 | | 43.337 | 1.00 | 42.71 | | | | С |
| | MOTA | 10379 | CZ2 | | | | 14.202 | 41.229 | 43.271 | | 45.71 | | | | C |
| | ATOM | 10381 | C . | | В 277 | | | 41.180 | 42.123 | | 48.22 | | | | 0 |
| | ATOM | 10382 | 0 | | В 277 | | 14.664 | | 44.184 | | 50.19 | | | | N |
| | MOTA | 10383 | N | | В 278 | | 14.594 | 40.388 | 43.918 | | | | | | С |
| 30 | MOTA | 10385 | CA | | B 278 | | 15.742 | 39.549 | | 1.00 | 53.84 | | | | c |
| | MOTA | 10387 | CB | | B 278 | | 16.264 | 39.003 | 45.227 | | | | | | č |
| | ATOM | 10390 | CG | | B 278 | | 15.300 | 38.046 | 45.876 | | 53.98 | | | | ŏ |
| | ATOM | 10391 | OD1 | ASN | в 278 | | 15.630 | 36.887 | 46.122 | _ | 58.86 | | | | |
| | MOTA | 10392 | ND2 | ASN | В 278 | | 14.095 | 38.528 | 46.162 | | 58.00 | • | | | N |
| 35 | ATOM | 10395 | С | ASN | В 278 | | 15.579 | 38.410 | 42.941 | | 47.96 | • | | | C |
|)) | MOTA | 10396 | ō | | В 278 | | 16.577 | 37.810 | 42.616 | | 48.00 | | | | 0 |
| | ATOM | 10397 | N | | В 279 | | 14.384 | 38.074 | 42.447 | | 48.44 | | | | N |
| | | 10399 | CA | TIF | В 279 | | 14.356 | 36.960 | 41.496 | 1.00 | 44.44 | | | | С |
| | MOTA . | | CB | | В 279 | | 13.006 | 36.227 | 41.370 | 1.00 | 48.45 | | | | С |
| 40 | MOTA | 10401 | | | В 279 | | 11.844 | 37.181 | | 1.00 | 53.39 | | | | С |
| 40 | MOTA | 10403 | CG. | 1 111E | В 279 | | 10.671 | 36.467 | | 1.00 | 49.91 | | | | С |
| | MOTA | 10406 | CD. | 1 111 | D 270 | | 12.724 | 35.335 | | | 0.44.38 | | ٠. | | C. |
| | MOTA | 10410 | | 7 TPE | В 279 | | 14.796 | 37.386 | | | 47.23 | | | | C |
| | MOTA | 10414 | С | | В 279 | | | 36.515 | | | 48.85 | | | | Ò |
| | ATOM | 10415 | | | В 279 | | 15.121 | | | | 51.85 | | | | N |
| 45 | MOTA | 10416 | | | В 280 | | 14.809 | 38.714 | | | 0 43.99 | | | | Ċ |
| | MOTA | 10418 | CA | | B 280 | | 15.181 | 39.313 | | | 0 47.60 | | | | c |
| | MOTA | 10420 | CB | | E B 280 | | 14.346 | | | | | | | | č |
| | ATOM | 10423 | CG | PHI | E B 280 | | 12.840 | | | | 0 50.69 | | | | č |
| | ATOM | | | 1 PH | ЕВ 280 | | 12.157 | 40.062 | | | 0 47.59 | | | | |
| 50 | MOTA | | | 1 PH | E B 280 | | 10.793 | 39.871 | | | 0 49.69 | | | | . C |
| 50 | MOTA | | | | Е В 280 | | 10.114 | 39.944 | 38.220 | | 0 53.43 | | | | C |
| | ATÓM | | | | E B 280 | | 10.792 | | 39.402 | 1.0 | 0 50.88 | | | | C |
| | | | | 2 DH | E B 280 | | 12.126 | | | 1.0 | 0 44.76 | | | | С |
| | MOTA | | | DII | E B 280 | | 16.604 | | | | 0 43.94 | | | | C |
| | ATOM | | | | E B 280 | | 17.114 | | | | 0 43.28 | | | | 0 |
| 55 | MOTA | | | | | • | | | | | 0 37.73 | | | | N |
| | ATOM | | | | O B 281 | | 17.256 | | | 3 1 0 | 0 33.44 | | | | С |
| | MOTA | | | . PR | O B 281 | | 18.668 | | | | 0 36.50 | | | | Č |
| • | ATOM | 10439 | CE | | O B 281 | | 19.089 | | | | 0 38.20 | | | | c |
| | ATOM | 10442 | CG | PR | O B 281 | | 18.034 | | | | | | | | c |
| 60 | ATOM | | CI |) PR | O B 281 | | 16.737 | | | | 0 39.79 | | | 2 | C |
| | ATOM | | | PR | O B 281 | | 18.928 | 3 41.34 | 6 37.03 | p 1.0 | 0 36.85 |) | | | ٠. ٠ |
| | | | | | • | | | | | | | | | | |

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PRO B 281
                                     18.039 41.984
                                                      36.537 1.00 43.97
5 ATOM 10449
                  0
          10450
                  N
                      VAL B 282
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                                              41.806
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                      VAL B 282
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                      VAL B 282
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                                                      37.809
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                  CB
    MOTA
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                                                              1.00 40.33
    ATOM
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                      VAL B 282
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                                                      35.184
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                                                                                    N
                      ILE B 283
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                      ILE B 283 ·
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           10468
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                                              44.748 32.505
                                                              1.00 40.29
                      ILE B 283 .
                                     20.505
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    MOTA
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                                     19.273
                                             43.855
                                                      32.531
                                                              1.00 35.95
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                                                              1.00 46.04
                                                                                    С
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                      ILE B 283
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                      SER B 284
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                                                      32.612
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                                                                                    N
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           10485
                  N
                      SER B 284
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                                                              1.00 46.53
                                                                                     C
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                      LEU B 285
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30
           10503
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                                     23.394
                                                      28.921
                                                              1.00 38.05
                                                                                     С
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                                                      28.300
                                                              1.00 35.50
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           10505
                  CD1 LEU B 285
     MOTA
           10509
                  CD2 LEU B 285
                                     22.717
                                              47.308
                                                      28.356
                                                              1.00 37.92
                                                                                     C
                                                                                     С
                                   27.330
                                              48.156
                                                      29.671 1.00 39.56
     ATOM
           10513
                  С
                      LEU B 285
                                     27.562 48.901
                                                      30.617
                                                              1.00 37.44
                                                                                     O
           10514
                      LEU B 285
     MOTA
                  0
35
     ATOM
           10515
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                      TYR B 286
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                                                              1.00 39.99
                                                                                    N
                                                              1.00 45.00
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                  CA
                      TYR B 286
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                                                      28.835
                                                                                     С
                      TYR B 286
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                                                      28.685
                                                               1.00 46.18
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                  CB
     MOTA
           10522
                  CG
                      TYR B 286
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                                              45.888
                                                      29.752
                                                               1.00 48.12
                                                                                     С
                                                               1.00 47.49
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                                                                                     C
     ATOM
           10523
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                                     29.678
                                                      29.975
40
                                              44.036
                                                               1.00 46.99
                                                                                     C
           10525
                  CE1 TYR B 286
                                     29.767
                                                      30.934
     MOTA
           10527
                      TYR B 286
                                     30.945
                                             43.911
                                                      31.667
                                                               1.00 49.87
                                                                                     С
     MOTA
                  CZ
           10528
                      TYR B 286
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                                              42.952
                                                      32.643
                                                               1.00 45.54
     MOTA
                  OH
     MOTA
           10530
                  CE2 TYR B 286
                                     31.986
                                             44.753
                                                      31.444
                                                               1.00 45.24
                                                                                     С
     MOTA
           10532
                  CD2 TYR B 286
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                                                      30.511
                                                              1.00 38.43
                                                                                     С
                                   29.917
45
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                                                      27.602
                                                               1.00 46.95
    MOTA
           10534
                      TYR B 286
                                                                                     C
                  С
                      TYR B 286
                                     29.613
                                             48.633
                                                      26.494
                                                              1.00 43.90
                                                                                     0
     ATOM
           10535
                  0
    · ATOM
           10536
                      LEU B 287
                                     30.480
                                              50.269
                                                      27.782
                                                               1.00 42.38
                                                                                     N
                  N
     ATOM
           10538
                  CA
                      LEU B 287
                                     30.526
                                              51.257
                                                      26.741
                                                               1.00 40.41
                                                                                     C
     MOTA
           10540
                      LEU B 287
                                      29.874
                                              52.562
                                                      27.203
                                                               1.00 39.65
                                                                                     C
                  CB
50
     MOTA
           10543
                  CG
                      LEU B 287
                                     28.487
                                              52.664
                                                      27.896
                                                               1.00 35.23
                                                                                     С
                                              53.994
                                                                                     C
     MOTA
           10545
                  CD1 LEU B 287
                                     28.344
                                                      28.625
                                                               1.00 37.04
                                              52.558
                                     27.480
                                                                                     С
     MOTA
           10549
                  CD2 LEU B 287
                                                      26.938
                                                               1.00 26.22
                                     31.960
                                              51.571
                                                      26.564
                                                               1.00 45.87
                                                                                     Ç
     MOTA
           10553
                  C ·
                      LEU B 287
     ATOM
           10554
                      LEU B 287
                                     32.716
                                              51.400
                                                      27.474
                                                               1.00 51.50
                                                                                     0
                  0
                                    32.356
55
     ATOM
           10555
                      MET B 288
                                              52.041
                                                      25.401
                                                               1.00 50.25
                                                                                     N
                  N
     ATOM
           10557
                      MET B 288
                                      33.749
                                              52.315
                                                      25.123
                                                               1.00 52.89
                  CA
     MOTA
           10559
                  CB
                      MET B 288
                                      33.884
                                              52.619
                                                      23.654
                                                               1.00 57.49
                                                                                     C
                                                                                     С
           10562
                                      35.255
                                             52.585
                                                      23.075
     MOTA
                  CG
                      MET B 288
                                                               1.00 59.46
                                                                                     s
     ATOM
           10565
                  SD
                      MET B 288
                                      35.108
                                              53.029
                                                      21.308
                                                               1.00 62.39
60
           10566
                                      35.316
                                              51.616
                                                      20.631
                                                                                     C
     ATOM
                  CE. MET B 288
                                                               1.00 56.14
     ATOM
           10570
                  С
                      MET B 288
                                      34.157
                                              53.518
                                                      25.927
                                                               1.00 55.91
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| | | | | | | | | | | 1 00 | C7 04 | | - | 0 |
|------|-------|--------|------|---------|---------|-----|--------|--------|--------|-------|---------|---|---|-----|
| 5 | ATOM | 10571 | | MET E | | | 33.354 | 54.433 | 26.109 | 1.00 | | | | N . |
| , | | | | | 3 289 | | 35.403 | 53.522 | 26.405 | 1.00 | | | | C |
| | | | | | 3 289 | | 35.911 | 54.608 | 27.230 | 1.00 | | | | C |
| | ATOM | 10577 | С | GLY. E | 3 289 | | 36.880 | 55.482 | 26.473 | 1.00 | | | | o . |
| | | | 0 | GLY E | 3 289 | | 37.113 | 55.267 | 25.286 | 1.00 | | | | Ŋ |
| 10 | ATOM | 10579 | N | GLU F | 3 290. | | 37.460 | 56.465 | 27.143 | | 57.96 | | | C |
| 10 | ATOM | 10581 | CA | GLU I | 3 290 | | 38.341 | 57.390 | 26.444 | | 59.77 | | | c |
| | ATOM | 10583 | СВ | | 3 290 | | 38.373 | 58.726 | 27.150 | 1.00 | 59.36 | | | c |
| | ATOM | 10586 | CG | | B 290 | | 37.021 | 59.394 | 27.100 | | 60.99 | | | C |
| | ATOM | 10589 | CD. | | в 290 | | 37.125 | 60.824 | 26.612 | | 63.85 | | | |
| 15 | ATOM | 10590 | | | В 290 | • | 37.333 | 61.687 | 27.500 | | 67.58 | | | 0 |
| 13 | ATOM | 10591 | OE2 | GLU I | в 290 | | 37.006 | 61.078 | 25.360 | | 50.86 | | | 0 |
| | | 10592 | ·C | | В 290 | | 39.767 | 56.919 | 26.220 | | 61.97 | | | С |
| | ATOM | 10592 | 0 | | B 290 | | 40.377 | 57.319 | 25.243 | 1.00 | 65.39 | | | 0 |
| • | MOTA | | N | VAI. | B 291 | | 40.325 | 56.086 | 27.090 | | 62.97 | | | N |
| - | ATOM | 10594 | CA | | B 291 | | 41.697 | 55.643 | 26.854 | | 61.83 | | | С |
| 20 | ATOM | 10596 | | | B 291 | | 42.336 | 55.119 | 28.158 | | 63.23 | | | C · |
| | MOTA | 10598 | CB | | B 291 | | 43.820 | 54.897 | 27.988 | | 67.30 | | | С |
| .*. | MOTA | 10600 | | | B 291 | | 42.121 | 56.153 | 29.281 | 1.00 | 66.27 | | | С |
| | ATOM: | 10604 | | | B 291 | | 41.452 | 54.644 | 25.731 | 1.00 | 59.22 | | | C, |
| | MOTA | 10608 | C | | | | 40.303 | 54.325 | 25.463 | 1.00 | 56.93 | | | 0 |
| 25 | MOTA | 10609 | 0 | | B 291 | | 42.468 | 54.169 | 25.038 | | 58.29 | | | N |
| | MOTA | 10610 | N | | B 292 | | 42.400 | 53.183 | 23.969 | | 59.67 | | | С |
| | MOTA | 10612 | CA | | B 292 | | 43.311 | 53.327 | 22.909 | | 62.91 | | | C |
| | MOTA | 10614 | CB | | B 292 | | 42.746 | 53.895 | 21.712 | | 63.26 | | | 0 |
| | ATOM | 10616 | OG1 | | B 292 | | 42.740 | 51.953 | | 1.00 | 62.53 | | | С |
| 30 | MOTA | 10618 | CG2 | | B 292 | | | 51.766 | 24.494 | 1.00 | 57.76 | | | С |
| | ATOM | 10622 | С | | B 292 | | 42.280 | | 25.393 | 1 00 | 57.85 | | | 0 |
| | MOTA | 10623 | 0 | | B 292 | | 43.004 | 51.517 | 23.968 | 1 00 | 61.18 | | | N |
| | MOTA | 10624 | N | | B 293 | | 41.535 | 50.819 | 24.428 | 1 00 | 66.82 | | | С |
| | MOTA | 10626 | CA | | В 293 | | 41.737 | 49.429 | 24.426 | i 00 | 71.42 | | | С |
| . 35 | MOTA | 10628 | CB | | В 293 | | 43.237 | 49.258 | 24.291 | | 73.25 | | | С |
| | MOTA | 10631 | CG | | В 293 | | 44.001 | 48.005 | 24.231 | | 76.24 | | | C |
| | MOTA | 10634 | CD | | В 293 | | 45.538 | 48.253 | 23.180 | | 73.24 | | | 0 |
| • | ATOM | 10635 | | | B 293 | | 46.178 | 47.731 | 25.015 | | 73.09 | | | N |
| | MOTA | 10636 | NE2 | | B 293 | | 46.111 | 49.048 | | | 66.33 | | | C |
| 40 | ATOM | 10639 | С | | B 293 | | 40.883 | 49.060 | | | 69.45 | | | 0 |
| | ATOM | 10640 | 0 | GLN | B 293 | | 40.602 | 47.896 | | | 64.46 | | | N |
| | MOTA | 10641 | N | | B 294 | • | 40.467 | | | | 57.83 | | | Ċ |
| | ATOM | 10643 | CA | | В 294 | | 39.810 | | | | 58.59 | | | c |
| | ATOM | | CB | GLN | B 294 | | 40.597 | | | | 57.32 | | | Č |
| 45 | ATOM | | CG | | . в 294 | • | 40.167 | | | | 62.05 | | | Č |
| | MOTA | | CD | | B 294 | • | 41.418 | | | | | | | Õ |
| | MOTA | | | | В 294 | • | 41.355 | | | | 72.12. | | | Ŋ |
| | ATOM | | NE | 2 GLN | B 294 | | 42.570 | | | | 0 60.53 | | | c |
| | ATOM | | | | B 294 | . • | 38.287 | | | | 57.84 | | | |
| . 50 | ATOM | | | | В 294 | | 37.830 | 51.216 | | 1.0 | 0 56.18 | | | - 0 |
| . 50 | ATOM | | | | В 295 | • | 37.490 | 49.580 | | | 0 54.23 | | | N |
| • | ATOM | | | | В 295 | | 36.050 | 49.896 | 28.573 | | 0 53.45 | | | C |
| | ATOM | _ | | | В 295 | | 35.178 | | | | 0 52.98 | | | . C |
| | | | | | R B 295 | | 35.006 | | | | 0 55.81 | • | | 0 |
| 55 | ATOM | | | | R B 295 | | 35.503 | | | | 0 49.98 | | | C |
| 55 | ATOM | | | | R B 295 | | 36.119 | | 30.832 | 1.0 | 0 47.16 | | | 0 |
| | ATOM | | | | E B 296 | | 34.34 | | 30.220 | | 0 48.76 | | | N |
| | ATOM | | | | E B 296 | | 33.70 | · | | 5 1.0 | 0 46.25 | | | С |
| | ATON | | | | B 296 | | 33.85 | | | | 0 45.49 | | | С |
| | MOTA | | | | E B 296 | | 32.90 | | | | 0 44.22 | | | С |
| 60 | | | | | E B 296 | | 31.72 | | | | 0 47.00 | | | . с |
| | ATON | M 1067 | , CL |) T EUI | D 230 | , | J1.72. | | | | | | | |

| 5 | MOTA | 10679 | CE1 | | B 296 | | 30.808 | 53.551 | 32.396 | 1.00 | | | | Ċ |
|------|--------------|----------------|--------|-----|----------------|----|--------|--------|--------|------|-------|---|---|-----|
| _ | ATOM | 10681 | CZ | | В 296 | | 31.089 | 54.394 | 31.341 | | 40.65 | | | C · |
| | ATOM | 10683 | | | B 296 | | 32.268 | 54.266 | 30.638 | 1.00 | | | | C |
| | ATOM. | 10685 | CD2 | PHE | В 296 | | 33.159 | 53.302 | 30.984 | 1.00 | | | | C |
| | ATOM | 10687 | C - | PHE | В 296 | | 32.232 | 49.871 | 31.423 | | 48.20 | | | С |
| 10 | ATOM | 10688 | 0 | PHE | B 296 | | 31.778 | 49.499 | 30.341 | | 54.42 | | | 0 |
| | ATOM | 10689 | N | ARG | В 297 | | 31.501 | 49.849 | 32.544 | 1.00 | 45.88 | | | N |
| | MOTA | 10691 | CA | ARG | B 297 | | 30.130 | 49.426 | 32.526 | 1.00 | 43.75 | | | С |
| | ATOM. | 10693 | | | В 297 | | 30.058 | 47.928 | 32.696 | | 46.61 | | | С |
| | ATOM | 10696 | CG | ARG | В 297 | | 30.812 | 47.407 | 33.875 | 1.00 | 52.65 | | | С |
| 15 | ATOM | 10699 | CD | | В 297 | ٠. | 30.556 | 45.919 | 34.138 | 1.00 | 52.49 | | | C |
| 1,5 | ATOM | 10702 | NE | | В 297 | | 30.710 | 45.525 | 35.546 | 1.00 | 51.81 | | | N |
| | ATOM | 10704 | CZ | | в 297 | | 31.212 | 44.358 | 35.939 | 1.00 | 48.75 | | | С |
| | ATOM | 10705 | | ARG | B 297 | | 31.614 | 43.487 | 35.042 | 1.00 | 53.62 | | | N |
| . • | ATOM | 10708 | | | B 297 | | 31.317 | 44.050 | 37.222 | 1.00 | 43.21 | | | N |
| 20 | ATOM. | 10711 | С | | B 297 | | 29.314 | 50.074 | 33.615 | 1.00 | 47.03 | | • | С |
| 20 | ATOM | 10712 | ō | | B 297 | | 29.852 | 50.469 | 34.676 | 1.00 | 48.02 | | | 0 |
| • | ATOM | 10713 | N | | B 298 | | 28.010 | 50.187 | 33.294 | 1.00 | 45.30 | | | N |
| | ATOM | 10715 | CA | | B 298 | | 26.937 | 50.674 | 34.150 | 1.00 | 44.58 | | | С |
| | ATOM | 10717 | CB | | B 298 | | 26.152 | 51.846 | 33.497 | 1.00 | 42.21 | | | С |
| 25 | ATOM | 10717 | | | B 298 | | | 51.391 | 32.217 | | 40.03 | | | C |
| 23 | ATOM | 10713 | | | B 298 | | 24.548 | 52.508 | 31.592 | | 39.09 | | | С |
| | ATOM | 10722 | | | B 298 | | 27.077 | 52.977 | 33.228 | 1.00 | 43.78 | | | С |
| | ATOM | 10720 | C | | B 298 | | 25.987 | 49.471 | 34.284 | | 45.83 | | | С |
| | | 10730 | 0 | | B 298 | | 25.735 | 48.749 | 33.325 | | 38.32 | | | 0 |
| 30 | MOTA | 10731 | N | | B 299 | | 25.443 | 49.270 | 35.467 | | 46.26 | | | N |
| .30 | ATOM | 10732 | CA | | B 299 | | 24.696 | 48.072 | 35.721 | | 47.54 | | | C |
| | MOTA | 10734 | | | B 299 | | 25.575 | 47.181 | 36.607 | | 52.72 | | | С |
| | ATOM | 10738 | | | B 299 | | 26.587 | 46.537 | 35.810 | | 52.36 | | | 0 |
| | ATOM | 10730 | | | B 299 | | 24.789 | 46.025 | 37.227 | | 53.54 | | | С |
| 35 | ATOM | 10740 | C | | B 299 | | 23.441 | 48.459 | 36.439 | | 47.53 | | | С |
| 33 | ATOM | 10744 | 0 | | B 299 | | 23.554 | 49.107 | 37.478 | | 45.39 | | • | 0 |
| | MOTA | | N | | B 300 | | 22.265 | 48.087 | 35.887 | | 47.99 | , | | N |
| | MOTA . | 10746 10748 | CA. | | В 300 | • | 20.952 | 48.367 | 36.518 | | 46.84 | | | · с |
| | ATOM | 10740 | CB | | В 300 | | 19.924 | 49.104 | 35.627 | | 46.77 | | | · C |
| 40 | MOTA MOTA | 10752 | | | B 300 | | 19.842 | 48.506 | 34.244 | | 45.61 | | | С |
| 40 | ATOM | 10755 | | | В 300 | | 18.475 | 48.734 | 33.633 | | 46.44 | | | С |
| - | MOTA | 10759 | | | В 300 | | 20.194 | 50.538 | 35.586 | _ | 52.09 | | | С |
| | ATOM | 10763 | C | | B 300 | * | 20.186 | 47.167 | 36.971 | | 44.73 | | | Ç |
| | ATOM | 10764 | Ö | | В 300 | | 20.413 | 46.046 | 36.543 | | 43.89 | | | Ó |
| 45 | - | 10765 | N | | B 301 | | 19.231 | 47.509 | 37.816 | | 46.21 | | | N |
| 43 | ATOM | 10767 | CA. | | B 301 | | 18.355 | 46.631 | 38.524 | | 44.01 | | • | . C |
| | ATOM | 10769 | CB. | | B 301 | | 18.303 | 47.094 | 39.973 | • | 47.01 | | | Č |
| | MOTA | 10703 | CG | | B 301 | | | 47.990 | | | 40.39 | | | С |
| | ATOM | | | | В 301 | | 19.093 | 48.496 | 41.828 | 1.00 | 40.91 | | | С |
| 50 | ATOM | 10774 | | | B 301 | | 20.671 | 47.123 | | | 47.03 | | | С |
| 50 | MOTA | 10778 10782 | ·C | | B 301 | | 16.936 | 46.740 | | | 46.44 | | | С |
| | ATOM | | | | B 301 | | 16.540 | 47.644 | 37.336 | | 43.22 | | | 0 |
| | ATOM | 10783 | 0 N | | B 302 | | 16.136 | 45.819 | | | 51.74 | | | N |
| | ATOM | 10784 | N | | | | 14.748 | 45.738 | 38.120 | | 47.89 | | | C |
| 55 . | ATOM | 10785 | CA | | B 302 B 302 | | 14.746 | 44.417 | | | 51.94 | | | č |
| 55 | ATOM | 10787 | CB | | B 302 | | 15.105 | 44.241 | 39.916 | | 53.36 | | | c |
| | ATOM | 10790 | .CG | | | | 16.475 | 44.793 | | | 53.46 | | | c |
| | ATOM | 10793 | CD | | B 302 | | 14.008 | | | | 43.06 | • | | Č |
| | ATOM | | С | | B 302 | | | | | | 42.92 | | | . 0 |
| 60 | ATOM | | 0 | | B 302 | | 12.940 | | | | 42.92 | | | N |
| 60 | ATOM | | N | GLN | B 303 | | 14.582 | | | | 42.11 | | | c |
| | MOTA | 10800 | CA | GLN | B 303 | | 13.930 | 40.707 | 40,233 | | 45.11 | • | | |

| | | | | | | | | | | | _ | | | _ |
|-----|--------|--------|-----|-------|----------------|---|--------|----------|--------|------|---------|---|---|-----|
| 5 | ATOM | 10802 | CB | GLN B | 303 | | 14.625 | 49.192 | 41.504 | | 40.42 | | | C · |
| , | ATOM | 10805 | CG | GLN B | | | 14.037 | 48.667 | 42.758 | | 40.53 | | | С |
| | ATOM | 10808 | CD | GLN B | | | 14.744 | 47.461 | 43.285 | | 43.06 | | | C |
| | MOTA | 10809 | | GLN B | | | 15.546 | 46.827 | 42.579 | | 39.84 | | | 0 |
| | ATOM | 10810 | | GLN B | | | 14.449 | 47.126 | 44.543 | | 43.69 | | | N |
| 10 | ATOM | 10813 | C | GLN B | | | 14.061 | 49.794 | 39.271 | 1.00 | 45.98 | | | C , |
| 10 | | 10813 | Ö | GLN B | | | 13.689 | 50.934 | 39.528 | 1.00 | 53.51 | | | 0 |
| | ATOM | 10815 | N | GLN B | | | 14.602 | 49.469 | 38.129 | 1.00 | 47.03 | | | N |
| | MOTA | 10817 | CA | GLN B | | | 14.815 | 50.478 | 37.174 | | 46.42 | | (| C. |
| | ATOM | | CB | GLN B | | | 16.294 | 50.534 | 36.921 | 1.00 | 48.97 | | | С |
| 1.5 | MOTA | 10819 | | GLN B | | | 16.894 | 51.900 | 37.204 | 1.00 | 45.42 | | | С |
| 15 | MOTA | 10822 | CG | GLN E | | | 17.282 | 52.050 | 38.613 | | 42.60 | | | С |
| | MOTA | 10825 | CD | | | | 16.869 | 52.990 | 39.271 | | 55.93 | | 4 | 0 |
| | MOTA | 10826 | OE1 | | | | 18.088 | 51.152 | 39.088 | | 43.68 | | | N |
| | MOTA | 10827 | | GLN E | | | 14.081 | 50.144 | 35.904 | | 51.85 | | | С |
| | MOTA | 10830 | C | GLN E | | | 13.344 | 51.021 | 35.361 | | 53.64 | | | 0 |
| 20 | MOTA | 10831 | 0 | GLN E | | | | 48.905 | 35.420 | | 49.13 | | | N |
| • | MOTA | 10832 | N | TYR E | | | 14.276 | 48.452 | 34.192 | | 48.73 | | | С |
| | ATOM | 10834 | CA | TYR E | | | 13.624 | | 33.409 | | 48.24 | • | | C |
| | MOTA | 10836 | CB | TYR F | | | 14.445 | 47.418 | 34.075 | | 45.68 | | | С |
| | MOTA | 10839 | CG | TYR E | | | 14.696 | 46.120 | | | 49.08 | | | Č |
| 25 | MOTA | 10840 | | TYR I | | | 13.829 | 45.057 | 33.906 | | 51.64 | | | Ċ |
| | MOTA | 10842 | | TYR I | | | 14.056 | 43.872 | 34.505 | | 59.15 | | | c |
| • | MOTA . | 10844 | CZ | | 3 305 | | 15.186 | | 35.301 | | 61.84 | | | ō |
| | ATOM | 10845 | OH | | 305 | | 15.454 | 42.500 | 35.932 | | | | | c |
| | MOTA | 10847 | | TYR I | | | 16.063 | 44.765 | 35.467 | | 56.26 | | | Ċ. |
| 30 | ATOM | 10849 | CD2 | TYR I | | | 15.805 | 45.948 | 34.857 | | 48.39 | | | C |
| | ATOM | 10851 | С | | В 305 | | 12.264 | 47.897 | 34.416 | | 51.41 | | | o |
| | MOTA | 10852 | 0 | TYR I | B 305 | | 11.637 | 47.411 | 33.467 | | 50.10 | | | И |
| | MOTA | 10853 | N | | В 306 | | 11.807 | 47.952 | 35.662 | | 51.83 | | | C |
| | MOTA | 10855 | CA | LEU | В 306 | | 10.481 | 47.474 | 35.996 | | 49.68 | | | c |
| 35 | ATOM | 10857 | CB | LEU 1 | В 306 | | 10.508 | 46.481 | 37.129 | | 52.01 | | | c |
| • | ATOM | 10860 | CG | | в 306 | | 10.687 | 45.019 | 36.827 | | 51.56 | | | c |
| | MOTA | 10862 | | LEU : | | | 10.108 | 44.267 | 38.015 | | 53.34 | | | c |
| | MOTA | 10866 | CD2 | LEU | в 306 | | 9.924 | 44.708 | 35.605 | | 56.13 | | | |
| | MOTA | 10870 | С | LEU | в 306 | | 9.884 | 48.717 | 36.499 | | 50.94 | | | C |
| 40 | MOTA | 10871 | 0 | LEU | в 306 | | 10.282 | 49.209 | 37.547 | | 50.28 | | | 0 |
| | MOTA | 10872 | N | ARG | в 307 | | 8.908 | 49.212 | 35.764 | | 49.70 | | | N |
| | ATOM | 10874 | CA | ARG | B 307 | | 8.419 | 50.538 | 35.974 | | 44.12 | | | C |
| | ATOM | 10876 | CB | ARG | в 307. | | 8.456 | 51.259 | 34.633 | | 38.83 | | | С |
| | ATOM | 10879 | CG | ARG | B 307 | • | 7.667 | 52.549 | 34.573 | | 42.47 | | | С |
| 45 | ATOM | 10882 | CD | | в 307 | | 7.695 | 53.176 | 33.188 | | 46.67 | | | C |
| •• | ATOM | .10885 | NE | | В 307 | • | 6.899 | 52.434 | 32.208 | | 49.09 | | | N |
| | . ATOM | 10887 | CZ | | B 307 | | 5.744 | 52.870 | | _ | 55.81 | | | С |
| | ATOM | 10888 | | 1 ARG | | | 5.245 | 54.035 | 32.116 | | 54.72 | , | | N |
| | ATOM | 10891 | NH | 2 ARG | В 307 | | 5.072 | 52.145 | 30.825 | | 58.11 | | | N |
| 50 | ATOM | | С | | B.307 | | 7.038 | 50.495 | 36.548 | | 46.97 | | | С |
| 50 | ATOM | | ŏ | | В 307 | | 6.218 | | 35.992 | 1.00 | 51.21 | | | 0 |
| | ATOM | | | | B 308 | _ | 6.799 | 51.239 | | | 0 46.48 | | | N |
| | ATOM | | CA | | B 308 | | 5.547 | | | | 0 50.59 | | | С |
| | | | | | B 308 | | 5.892 | | | | 0 48.57 | | | С |
| 55 | MOTA | | | | B 308 | | 7.261 | | | 1.0 | 0 49.01 | | | С |
| 55 | MOTA | | | | B 308 | | 7.773 | | | | 0 50.08 | | | С |
| | ATOM | | | | B 308 | | 4.465 | | | | 0 59.61 | • | | С |
| | ATOM | | | | B 308 | | 4.792 | | | | 0 64.89 | | | 0 |
| | ATOM | | | | | | 3.200 | | | | 0 62.04 | | | N |
| | MOTA | | | | B 309 B 309 | | 2.026 | | | | 0 64.12 | | | С |
| 60 | MOTA | | | | | | 1.720 | | | | 0 65.00 | • | | С |
| | MOTA | 10914 | CB | VAL | В 309 | | 1.,20 | . 01.001 | 55.550 | | | | | |

| | | <u>.</u> | | | | | | | | | - |
|-----|--------------|----------------|---------|-----|----------------|---|------------------|------------------|------------------|--------------------------|--------|
| 5 | ATOM | 10916 | CG1 | VAL | B 309 | | 2.994 | 51.101 | 35.294 | 1.00 63.78 | С |
| | ATOM | 10920 | CG2 | VAL | B 309 | | 0.825 | 50.415 | 36.150 | 1.00 64.85 | С |
| | ATOM | 10924 | С | VAL | B 309 | | 0.810 | 52.137 | 38.173 | 1.00 64.34 | С |
| | ATOM | 10925 | 0 | VAL | B 309 | | 0.764 | 51.261 | 39.002 | 1.00 55.43 | 0 |
| | ATOM | 10926 | N | | B 310 | | -0.215 | 52.936 | 37.977 | 1.00 70.92 | N |
| 10 | ATOM | 10928 | CA | GLU | B 310 | | -1.368 | 52.762 | 38.834 | 1.00 74.98 | . С |
| • | MOTA | 10930 | CB | GLU | B 310 | | -2.380 | 53.877 | 38.651 | 1.00 76.84 | С |
| | ATOM | 10933 | CG | GLU | B 310 | | -3.286 | 54.103 | 39.862 | 1.00 82.90 | C |
| * . | MOTA | 10936 | CD | | B 310 | | -2.610 | 53.829 | 41.205 | 1.00 84:06 | С |
| | ATOM | 10937 | OE1 | | B 310 | | -2.619 | 52.653 | 41.631 | 1.00 90.22 | 0 |
| 15 | MOTA | 10938 | OE2 | GLU | В 310 | | -2.082 | 54.774 | 41.841 | 1.00 83.28 | 0 |
| | ATOM | 10939 | С | GLU | B 310 | | -1.978 | 51.443 | 38.473 | 1.00 76.13 | C |
| | ATOM | 10940 | О | | B 310 | | ~1.908 | 51.029 | 37.296 | 1.00 76.20 | 0 |
| | ATOM | 10941 | N | | B 311 | | -2.558 | 50.766 | 39.470 | 1.00 78.57 | N |
| | ATOM | 10943 | CA | | В 311 | | -3.306 | 49.539 | 39.182 | 1.00 82.17 | С |
| 20 | MOTA | 10945 | CB | | B 311 | | -3.558 | 48.684 | 40.441 | 1.00 82.68 | С |
| | MOTA | 10948 | CG | | В 311 | | -3.918 | 47.211 | 40.111 | 1.00 83.41 | C |
| | MOTA | 10949 | | | B 311 | | -4.210 | 46.905 | 38.926 | 1.00 86.04 | 0 |
| | MOTA | 10950 | | | B 311 | | -3.931 | 46.295 | 40.976 | 1.00 76.70 | . 0 |
| 0.5 | ATOM | 10951 | C | | B 311 | | -4.643 | 49.948 | 38.570 | 1.00 83.78 | C |
| 25 | MOTA | 10952 | 0 | | B 311 | | -5.174 | 51.026 | 38.867 | 1.00 81.54 | 0 |
| | MOTA | 10953 | N | | B 312 | | -5.172 | 49.100 | 37.707 | 1.00 85.51 | N |
| | ATOM | 10955 | CA | | B 312 | | -6.496 | 49.341 | 37.181 | 1.00 88.99 | C |
| | ATOM | 10957 | CB | | B 312 | | -7.065 | 48.064 | 36.499 | 1.00 88.37 | C |
| 30 | ATOM. | 10959 10963 | | | B 312 | - | -8.222 | 48.405 47.356 | 35.595 | 1.00 88.24 | C |
| 30 | ATOM ATOM | 10967 | CGZ | | B 312 B 312 | | -5.979 -7.361 | 49.769 | 35.697 38.383 | 1.00 88.52 1.00 92.51 | c |
| | ATOM | 10968 | o | | B 312 | | -7.811 | 50.910 | 38.482 | 1.00 94.93 | 0 |
| | ATOM | 10969 | | | B 313 | | -7.563 | 48.866 | 39.331 | 1.00 96.03 | N |
| | ATOM | 10971 | CA | | B 313 | | -8.432 | 49.151 | 40.470 | 1.00 97.31 | c |
| 35 | ATOM | 10973 | CB | | B 313 | | -8.438 | 47.916 | 41.424 | 1.00 95.55 | c |
| | ATOM | 10977 | C | | В 313 | | -8.055 | 50.404 | 41.281 | 1.00 98.18 | Č |
| | ATOM | 10978 | 0 | | В 313 | | -8.868 | 50.852 | 42.088 | 1.00102.35 | 0 |
| | ATOM | 10979 | N | THR | B 314 | | -6.864 | 50.971 | 41.033 | 1.00 97.48 | N |
| * | MOTA | 10981 | CA | THR | B 314 | | -6.102 | 51.818 | 42.013 | 1.00 96.57 | С |
| 40 | MOTA | 10983 | CB | THR | B 314 | | -6.505 | 53.356 | 42.037 | 1.00 95.77 | С |
| | ATOM | 10985 | OG1 | | B 314 | | -7.547 | 53.635 | 42.985 | 1.00 95.94 | 0 |
| | ATOM | 10987 | | | B 314 | | -7.040 | 53.811 | 40.662 | 1.00 95.13 | С |
| : | ATOM | 10991 | C, | | B 314 | | -6.028 | 51.095 | 43.417 | 1.00 94.99 | С |
| 45 | ATOM | 10992 | 0 | | B 314 | | -6.148 | 51.703 | 44.505 | 1.00 89.26 | 0 |
| 45 | ATOM | 10993 | N | | B 315 | | -5.810 | 49.767 | 43.307 | 1.00 94.79 | N . |
| | ATOM | | CA | | B 315 | | -5.731 | 48.796 | 44.424 | 1.00 93.42 | C |
| | ATOM | 10997 | CB | | B 315 | | -5.712 | 47.335 | 43.911 | 1.00 93.27 | C |
| | ATOM | 11000 | OG | | B 315 | | -4.568 | 47.043 | 43.118 | 1.00 85.86 | 0 |
| 50 | MOTA | 11002 | C | | B 315 | | -4.516 | 49.033 | | 1.00 93.27 | c |
| 50 | ATOM | 11003 | 0 | | B 315 | | -3.681 | 49.893 48.279 | 44.995 | 1.00 94.12 | 0 |
| , | ATOM ATOM | 11004 11006 | N CA | | B 316 B 316 | | -4.410 -3.318 | 48.533 | 46.404 47.354 | 1.00 91.57 1.00 91.29 | ท C |
| | ATOM | 11008 | CB | | B 316 | | -3.756 | 48.294 | 48.839 | 1.00 91.29 | c |
| • | ATOM | 11011 | CG | | B 316 | | -4.329 | 49.622 | 49.500 | 1.00 93.01 | č |
| 55 | ATOM | 11014 | CD | | B 316 | | -4.619 | 49.576 | 51.022 | 1.00 91.31 | · c |
| | ATOM | 11015 | | | B 316 | | -4.691 | 48.505 | 51.626 | 1.00 90.86 | Ö |
| | ATOM | 11016 | NE2 | | B 316 | | -4.791 | 50.762 | 51.629 | 1.00 89.33 | N |
| | ATOM | 11019 | C | | B 316 | | -2.010 | 47.823 | 46.923 | 1.00 85.48 | c |
| | ATOM | | 0 | | B 316 | | -0.926 | 48.158 | | 1.00 84.70 | Ö |
| 60 | ATOM | 11021 | N | | B 317 | | -2.129 | 46.872 | 46.001 | 1.00 78.17 | N |
| | MOTA | 11023 | CA | | B 317 | | -0.980 | 46.180 | 45.434 | 1.00 76.19 | C |
| | | | | | | | | | | | |

| - 5 | ATOM | 11025 | CB | ASP | В | 317 | -1.492 | 45.121 | 44.472 | 1.00 73.46 | | | С |
|------|------|-------|-----|-----|---|-----|--------|--------|--------|------------|----|-----|---|
| • | ATOM | 11028 | CG | ASP | В | 317 | -2.262 | 44.078 | 45.184 | 1.00 72.17 | | | С |
| | ATOM | 11029 | OD1 | ASP | | | -2.407 | 44.252 | 46.424 | 1.00 70.34 | | | o |
| | MOTA | 11030 | OD2 | ASP | В | 317 | -2.743 | 43.073 | 44.620 | 1.00 70.32 | | | 0 |
| | ATOM | 11031 | С | ASP | | | 0.034 | 47.099 | 44.728 | 1.00 76.88 | | | C |
| 10 | ATOM | 11032 | 0 | | | 317 | -0.247 | 48.268 | 44.447 | 1.00 82.57 | | | ō |
| | ATOM | 11033 | N | | | 318 | 1.216 | 46.558 | 44.448 | 1.00 74.00 | | | N |
| | ATOM | 11035 | CA | ASP | | | 2.304 | 47.312 | 43.838 | 1.00 68.80 | | | C |
| | MOTA | 11037 | СВ | ASP | | | 3.577 | 47.191 | 44.686 | 1.00 70.82 | | | c |
| | ATOM | 11040 | CG | ASP | | | 3.534 | 48.035 | 45.962 | 1.00 71.07 | | | c |
| 15 | ATOM | 11041 | | ASP | | | 4.185 | 47.662 | 46.968 | 1.00 70.80 | | | ō |
| | ATOM | 11042 | | ASP | | | 2.884 | 49.087 | 46.052 | 1.00 73.30 | | | o |
| | ATOM | | ··C | ASP | | | 2.511 | 46.719 | 42.455 | 1.00 65.62 | | | c |
| | ATOM | 11044 | ŏ | ASP | | | 3.019 | 45.608 | 42.319 | 1.00 60.87 | | | Ö |
| | ATOM | 11045 | | CYS | | | 2.126 | 47.456 | 41.419 | 1.00 61.57 | • | | N |
| 20 | ATOM | 11047 | CA | | | 319 | 2.120 | 46.872 | 40.093 | 1.00 57.97 | • | | C |
| 20 | ATOM | 11049 | СВ | CYS | | | 0.736 | 46.962 | 39.463 | 1.00 57.57 | | | C |
| | ATOM | 11052 | SG | CYS | | | -0.613 | 46.137 | 40.403 | 1.00 68.12 | | • | s |
| | ATOM | 11052 | C | CYS | | | 3.220 | 47.524 | 39.269 | 1.00 52.64 | | | |
| | ATOM | 11053 | Ö | CYS | | | 3.745 | 48.540 | | 1.00 52.88 | | | C |
| 25 | ATOM | 11054 | | TYR | | | 3.745 | | 39.662 | | | | 0 |
| 23 | | | N | | | | | 46.945 | 38.130 | 1.00 47.04 | | | N |
| | MOTA | 11057 | CA | | | 320 | 4.728 | 47.385 | 37.415 | 1.00 50.79 | - | | C |
| | MOTA | 11059 | CB | TYR | | | 6.042 | 46.773 | 38.010 | 1.00 51.87 | | | C |
| | ATOM | 11062 | CG | TYR | | | 6.341 | 47.116 | 39.469 | 1.00 44.28 | | | С |
| 20 | MOTA | 11063 | | TYR | | | 5.861 | 46.331 | 40.512 | 1.00 51.75 | | | С |
| 30 | MOTA | 11065 | | TYR | | | 6.125 | 46.637 | 41.826 | 1.00 48.81 | | | С |
| | MOTA | 11067 | CZ | TYR | | | 6.873 | 47.737 | 42.090 | 1.00 51.67 | | | С |
| | ATOM | 11068 | OH | TYR | | | 7.161 | 48.090 | 43.379 | 1.00 63.11 | | | 0 |
| | ATOM | 11070 | | TYR | | | 7.351 | 48.512 | 41.073 | 1.00 46.32 | | | C |
| 35 | ATOM | 11072 | | TYR | | | 7.082 | 48.188 | 39.779 | 1.00 35.82 | | | С |
| 33 | ATOM | 11074 | С | TYR | | | 4.626 | 46.882 | 36.016 | 1.00 52.12 | | | С |
| | ATOM | 11075 | 0 | TYR | | | 4.082 | 45.809 | 35.792 | 1.00 56.07 | | | 0 |
| | ATOM | 11076 | N | LYS | | | 5.164 | 47.667 | 35.085 | 1.00 53.09 | | | N |
| | ATOM | 11078 | CA | LYS | | | 5.216 | 47.294 | 33.708 | 1.00 51.68 | • | | С |
| 40 . | ATOM | 11080 | CB | LYS | | | 4.684 | 48.430 | 32.832 | 1.00 57.10 | | | C |
| 40 | MOTA | 11083 | CG | LYS | | | 3.102 | 48.538 | 32.635 | 1.00 61.86 | | | С |
| | ATOM | 11086 | CD | LYS | | | 2.727 | 49.287 | 31.269 | 1.00 67.16 | | | С |
| | ATOM | 11089 | CE | LYS | | | 1.532 | 50.345 | 31.323 | 1.00 70.93 | | | С |
| | ATOM | 11092 | NZ | LYS | | | 1.847 | 51.846 | 31.459 | 1.00 71.64 | | | N |
| 45 | MOTA | 11096 | С | LYS | | | 6.681 | 47.049 | 33.421 | 1.00 49.27 | | | С |
| .43 | ATOM | 11097 | 0 | LYS | | | 7.544 | 47.694 | 33.987 | | | | 0 |
| | ATOM | | · N | PHE | | | 6.961 | 46.083 | 32.568 | 1.00 45.37 | •• | | N |
| • | ATOM | 11100 | CA | PHE | | | 8.291 | 45.825 | | 1.00 45.16 | | | С |
| | ATOM | 11102 | | PHE | | | | 44.478 | | 1.00 41.79 | | | C |
| 50 | ATOM | 11105 | CG | | | | 9.528 | 43.929 | 30.875 | 1.00 42.80 | | • • | С |
| 50 | | 11106 | | PHE | | | 10.627 | 43.747 | 31.697 | 1.00 41.54 | | ٠. | С |
| | MOTA | 11108 | | PHE | | | 11.812 | 43.202 | 31.188 | 1.00 46.06 | | | С |
| • | ATOM | 11110 | | PHE | | | 11.895 | 42.839 | 29.861 | 1.00 44.89 | | | С |
| | MOTA | 11112 | | PHE | | | 10.803 | 43.031 | 29.042 | 1.00 34.54 | | | С |
| | MOTA | 11114 | CD2 | PHE | В | 322 | 9.633 | 43.549 | 29.547 | 1.00 37.25 | | | С |
| 55 | MOTA | 11116 | C | PHE | | | 8.606 | 46.957 | 31.087 | 1.00 48.75 | • | | С |
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| | ATOM | 11122 | CB | ALA | В | 323 | 10.314 | 50.060 | 31.172 | 1.00 46.63 | | | С |
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                                    25.389
                                             60.268
                      TYR B 342
     MOTA
           11396
                  0
                                                                                   N
                                                             1.00 41.14
                                    23.952
                                             61.690
                                                     34.665
                      VAL B 343
           11397
     MOTA
                  N
                                                             1.00 38.62
                                    24.592
                                             61.717
                                                      33.333
                      VAL B 343
           11399
                  .CA
     MOTA
                                                     32.277
                                                             1.00 38.70
                                    23.618
                                             61.281
                      VAL B 343 ·
                  CB
     MOTA
           11401
                                             61.080
                                                      30.981
                                                             1.00 40.70
                  CG1 VAL B 343
                                     24.369
30
     MOTA
           11403
                                             59.960
                                                             1.00 42.16
                                                      32.703
                  CG2 VAL B 343
                                     22.943
           11407
     MOTA
                                                             1.00 36.25
                                     25.070
                                             63.099
                                                      32.869
     MOTA
           11411
                  С
                      VAL B 343
                                             64.079
                                                      32.905
                                                             1.00 43.95
                                     24.319
                      VAL B 343
     MOTA
           11412
                                                             1.00 37.32
                      VAL B 344
                                     26.305
                                             63.192
                                                      32.393
     MOTA
           11413
                  N
                                                      31.990
                                                             1.00 29.38
                                                                                   C
                                     26.868
                                              64.477
35
                      VAL B 344
           11415
                  CA
     MOTA
                                                      32.583
                                                             1.00 30.42
                      VAL B 344
                                              64.693
                                     28.183
     ATOM
           11417
                  CB
                                              66.115
                                                     32.541
                                                             1.00 36.77
                  CG1 VAL B 344
                                     28.516
           11419
     MOTA
                                                     34.036
                                                                                   С
                                                             1.00 38.24
                                              64.296
           11423
                  CG2 VAL B 344
                                     28.156
     MOTA
                                                                                   C
                                                      30.545 1.00 31.36
                                     27.087
                                              64.507
                      VAL B 344
     MOTA
           11427
                  С
                                                                                   O
                                              63.618
                                                      30.003 1.00 36.95
                      VAL B 344
                                     27.722
40
     MOTA
           11428
                  0
                                                             1.00 38.83
                                              65.555
                                                     29.935
                      PHE B 345
                                     26.543
           11429
     MOTA
                  N
                                                     28.494
                                                             1.00 41.14
                                             65.855
                      PHE B 345
                                      26.611
     MOTA
           11431
                  CA
                                   25.217
                                                      27.962
                                                              1.00 41.42
                                              66.193
                      PHE B 345
     MOTA
           11433
                  CB
                                                      28.278
                                                              1.00 44.84
                                     24.189
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           11436
                   CG
                      PHE B 345
     MOTA
                                                                                   С
                                                      27.366
                                                              1.00 42.09
                                      23.861
                                              64.165
45
           11437
                   CD1 PHE B 345
     MOTA
                                                                                   С
                                                      27.669
                                                              1.00 34.11
                                      22.953
                                              63.237
                  CE1 PHE B 345
     MOTA
           11439
                                                              1.00 41.08
                                   22.320
                                              63.238
                                                      28.870
                  CZ PHE B 345
     MOTA
           11441
                                                      29.785
                                                              1.00 46.16
                                              64.181
           11443
                  CE2 PHE B 345
                                      22.617
     MOTA
                                                              1.00 43.84
                                                      29.495
                                      23.551
                                              65.136
                  CD2. PHE B 345
     MOTA
           11445
                                      27.590
                                                      28.227
                                                              1.00 44.97
                                              67.007
50
           11447
                      PHE B 345
     MOTA
                   С
                                                                                   0
                                              68.145
                                                      28.007
                                                              1.00 43.88
                                   27.217
     MOTA
           11448
                   0
                       PHE B 345
                                                                                   N
                                                      28.241
                                                              1.00 47.40
                                     28.852
                                              66.609
                       ASP B 346
     MOTA
           11449
                   N
                                                                                   C
                                      30.032
                                              67.436
                                                      28.149
                                                              1.00 48.51
     ATOM
           11451
                   CA
                      ASP B 346
                                                     28.833
                                                                                   C
                                      31.139
                                              66.623
                                                              1.00.52.73
                      ASP B 346
     MOTA
           11453
                   CB
                                              67.433
                                                      29.321
                                                              1.00 60.43
55
                      ASP B 346
                                      32.313
           11456
                   CG
     ATOM
                                                      28.982
                                                              1.00 69.63
                                      32.437
                                              68.640
                   OD1 ASP B 346
     MOTA
            11457
                                      33.173
                                              66.892
                                                      30.074
                                                              1.00 54.36
                   OD2 ASP B 346
     MOTA
            11458
                                                      26.668
                                                             1.00 47.09
                                      30.301
                                              67.629
                       ASP B 346
     ATOM
            11459
                   С
                                                      26.076
                                                              1.00 45.68
                       ASP B 346
                                      31.160
                                              66.996
     MOTA
            11460
                   0
                                      29.506
                                              68.517
                                                      26.081
                                                              1.00 47.52
                       ARG B 347
60
     MOTA
            11461 N
                                      29.637
                                              68.935
                                                      24.701
                                                              1.00 43.73
                      ARG B 347
      MOTA
           11463
                  CA
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| | | | | | | | | | • | | | | | |
|-----|--------------|----------------|---------|-------|----------------|---|------------------|------------------|------------------|-------|--------------------|----|---|--------|
| 5 | »mom | 11465 | СВ | ARG I | 3 347 | | 28.570 | 69.962 | 24.423 | 1.00 | 43.30 | | | С |
| 5 | ATOM ATOM | 11468 | CG | | 3 347 | | 27.202 | 69.356 | 24.324 | | 42.11 | | | С |
| | ATOM | 11471 | CD | | 3 347 | | 26.079 | 70.326 | 24.660 | | 46.02 | | | С |
| | ATOM | 11474 | NE | | 3 347 | | 25.906 | 71.409 | 23.697 | | 46.95 | | | N |
| | ATOM | 11476 | CZ | | 3 347 | | 25.579 | 71.248 | 22.418 | | 49.44 | | | C |
| 10 | MOTA | 11477 | | ARG I | | | 25.401 | 70.035 | 21.910 | | 48.15 | | | N |
| 10 | ATOM | 11480 | | ARG I | | | 25.433 | 72.313 | 21.632 | | 51.53 | | | N |
| | ATOM | 11483 | С | | В 347 | | 30.988 | 69.558 | 24.396 | | 48.71 | | | C. |
| • | ATOM | 11484 | 0 | | в 347 | | 31.492 | 69.455 | 23.286 | | 49.46 | | | N |
| | ATOM | 11485 | N | | в 348 | | 31.578 | 70.217 | 25.379 | | 49.23 | | | C |
| 15 | ATOM | 11487 | CA | ALA | B 348 | | 32.842 | 70.875 | 25.172 | | 46.88 | | | Ċ |
| | ATOM | 11489 | CB | | В 348 | | 33.226 | 71.682 | 26.425 | | 48.10 53.46 | | | Ċ. |
| | MOTA | 11493 | С | | B 348 | | 33.901 | 69.837 | 24.849 | | 54.08 | | | ŏ |
| | MOTA | 11494 | 0 | | В 348 | | 34.834 | 70.103 | 24.076 | | 54.97 | | | N |
| | MOTA | 11495 | N | | В 349 | | 33.768 | 68.641 | 25.426 25.178 | | 51.50 | | | C |
| 20 | MOTA | 11497 | CA | | В 349 | | 34.773 | 67.599 | 26.517 | | 50.57 | | | Ċ |
| • | ATOM | 11499 | CB | | в 349 | | 35.395 | 67.153 | 27.060 | | 50.96 | | | C |
| | MOTA | 11502 | CG | | B 349 | | 36.426 | 68.192 67.948 | 28.466 | | 53.35 | | | C |
| | MOTA | 11505 | CD | | B 349 | | 36.963 | 66.891 | 28.506 | | 58.63 | | | N |
| | MOTA | 11508 | NE | | B 349 | | 37.988 | 66.554 | 29.599 | | 60.78 | | | С |
| 25 | MOTA | 11510 | CZ | | B 349 | | 38.667 38.427 | 67.189 | 30.747 | | 54.92 | | | N |
| | MOTA | 11511 | | | B 349 | | 39.585 | 65.593 | 29.545 | | 61.55 | | | N |
| | ATOM | 11514 | | | B 349 | | 34.290 | 66.413 | 24.305 | | 50.33 | | : | C. |
| | ATOM | 11517 | C: | | B 349 B 349 | | 34.994 | | 24.150 | | 50.96 | | | Ö |
| 20 | MOTA | 11518 | 0 | | B 350 | | 33.103 | 66.532 | 23.724 | | 46.02 | ٠. | | N |
| 30 | ATOM | 11519 | N CA | | В 350 | - | 32.610 | 65.465 | 22.881 | 1.00 | 46.35 | | | С |
| | MOTA | 11521 | CB | | В 350 | | 33.496 | 65.367 | 21.601 | 1.00 | 49.69 | | | С |
| | MOTA | 11523 11526 | CG | | B 350 | • | 33.014 | 64.434 | 20.402 | | 58.03 | | | С |
| • | MOTA MOTA | 11529 | CD | | В 350 | | 33.785 | 64.714 | 19.003 | | 58.14 | | | С |
| 35 | ATOM | 11532 | CE | | B 350 | | 33.246 | 63.860 | 17.760 | | 60.61 | | | С |
| 33. | ATOM | 11535 | NZ | | в 350 | | 33.683 | 64.245 | | | 56.11 | | | N |
| | ATOM | 11539 | С | | в 350 | | 32.554 | 64.164 | 23.717 | | 44.86 | | | C |
| | ATOM | 11540 | O. | | В 350 | | 32.810 | 63.100 | 23.206 | | 48.76 | | | 0 |
| | ATOM | 11541 | N | | B 351 | | 32.200 | 64.257 | 25.007 | | 44.60 | | | И С |
| 40 | ATOM | 11543 | CA | | В 351 | | 32.015 | 63.060 | 25.863 | |) 44.48 | | | c |
| | MOTA | 11545 | CB | | B 351 | | 33.225 | | 26.743 | | 0 43.82 | | | č |
| | MOTA | 11548 | CG | | В 351 | | 33.540 | | 27.571 | | 0 45.18 0 40.95 | | | č |
| | MOTA | 11551 | CD | | B 351 | | 34.789 | | 28.392 | _ | 0 46.55 | • | | N |
| | ATOM | 11554 | NE | | B 351 | | 34.687 | | | | 0 43.31 | | | C |
| 45 | MOTA | 11556 | . CZ | | B 351 | | 35.630 | | | | 0 41.89 | | | N |
| | MOTA | 11557 | | | B 351 | | 36.756 | | | | 0 54.20 | | | N |
| | · ATOM | | | 2 ARG | B 351 | | 35.456 | | | | 0 41.64 | | | С |
| | MOTA | | | | B 351 | | 30.791 | | | | 0 50.18 | | | . 0 |
| | MOTA | | | | B 351 | | 30.368 30.257 | | | | 0 38.69 | ٠. | | Ņ |
| 50 | MOTA | | | | B 352 | | 29.130 | | | | 0 45.01 | | | C |
| | MOTA | | | | B 352 | • | 28.098 | | | | 0 49.66 | • | | С |
| | MOTA | | | | B 352 B 352 | | 27.315 | | | | 0 52.66 | | | C |
| | ATOM | | | | B 352 | | 26.048 | | | 1.0 | 0 56.74 | | | С |
| | ATOM | | | | B 352 | | 27.127 | | | | 0 52.33 | | | С |
| 55 | ATOM | | | | В 352 | | 29.550 | | | | 0 46.49 | | • | С |
| | ATOM | | | | B 352 | | 30.129 | | | | 0 45.55 | | | 0 |
| | ATOM | | | | B 353 | | 29.237 | | | 1.0 | 0 46.26 | | | N |
| | ATOM | | | | В 353 | | 29.635 | | | 1.0 | 0 44.22 | | | . C |
| 60 | ATOM ATOM | | | | B 353 | | 28.530 | 60.101 | L 32.472 | | 0 40.63 | | | C |
| UU | MOTA MOTA | | | | B 353 | | 27.45 | | | 3 1.0 | 0 50.25 | | | 0 |
| | ATOR | | | | | • | | | | | | | | |

| • | | 1 | | | | | | | | | 13 |
|-----|------|----------------|----------|-------------|---|--------|--------|--------|------------|-----|-----|
| 5 | MOTA | 11591 | N | PHE B 354 | | 28.815 | 58.960 | 33.096 | 1.00 41.57 | | N |
| J . | ATOM | 11593 | CA | PHE B 354 | | 27.860 | 58.254 | 33.937 | 1.00 35.69 | | C |
| | ATOM | 11595 | СВ | PHE B 354 | | 27.614 | 56.866 | 33.365 | 1.00 42.54 | | C |
| | ATOM | 11598 | CG | PHE B 354 | | 27.032 | 56.890 | 31.992 | 1.00 48.12 | | C |
| | ATOM | 11599 | | PHE B 354 | | 27.843 | 57.064 | 30.896 | 1.00 47.79 | | С |
| 10 | | 11601 | | PHE B 354 | | 27.311 | 57.107 | 29.652 | 1.00 53.15 | | С |
| 10 | MOTA | 11603 | CZ | PHE B 354 | | 25.957 | 56.971 | 29.486 | 1.00 51.31 | | C |
| | MOTA | | | PHE B 354 | | 25.146 | 56.790 | 30.572 | 1.00 45.30 | | С |
| | ATOM | 11605 | | PHE B 354 | | 25.670 | 56.757 | 31.809 | 1.00 42.69 | | C |
| • | MOTA | 11607 | | | | 28.418 | 58.065 | 35.324 | 1.00 37.73 | | C |
| | ATOM | 11609 | С | PHE B 354 | | 29.561 | 57.648 | 35.479 | 1.00 36.56 | | 0 |
| 15 | MOTA | 11610 | 0 | PHE B 354 | | | 58.364 | 36.333 | 1.00 34.99 | | N |
| | ATOM | 11611 | N | ALA B 355 | | 27.611 | 58.081 | 37.695 | 1.00 31.85 | • | С |
| | MOTA | 11613 | CA | ALA B 355 | | 27.973 | | | 1.00 35.10 | | . C |
| | ATOM | 11615 | CB | ALA B 355 | | 28.631 | 59.305 | 38.285 | 1.00 33.10 | | C |
| | ATOM | 11619 | C | ALA B 355 | | 26.740 | 57.630 | 38.531 | | | Ö |
| 20 | ATOM | 11620 | O. | ALA B 355 | | 25.641 | 58.105 | 38.363 | 1.00 38.79 | | N |
| • | MOTA | 11621 | N | VAL B 356 | | 26.909 | 56.686 | 39.430 | 1.00 36.60 | | C |
| | MOTA | 11623 | CA | VAL B 356 | • | 25.801 | 56.261 | 40.272 | 1.00 35.07 | | c |
| | ATOM | 11625 | CB | VAL B 356 | | 26.370 | 55.348 | 41.344 | 1.00 32.99 | • | |
| | ATOM | 11627 | CG1 | VAL B 356 | | 25.358 | 55.012 | 42.383 | 1.00 38.64 | | C |
| 25 | MOTA | 11631 | CG2 | VAL B 356 | | 26.829 | 54.112 | 40.710 | 1.00 35.78 | | C · |
| 23 | MOTA | 11635 | С | VAL B 356 | | 25.077 | 57.477 | 40.879 | 1.00 35.09 | | C |
| | MOTA | 11636 | ō | VAL B 356 | | 25.717 | 58.401 | 41.338 | 1.00 40.54 | | 0 |
| | ATOM | 11637 | N | SER B 357 | | 23.752 | 57.483 | 40.905 | 1.00 41.74 | | N |
| | ATOM | 11639 | CA | SER B 357 | | 22.999 | 58.670 | 41.346 | 1.00 41.57 | | С |
| 30 | | 11641 | CB. | | | 21.721 | 58.803 | 40.523 | 1.00 47.83 | | С |
| 30 | MOTA | 11644 | OG . | SER B 357 | | 21.001 | 60.008 | 40.844 | 1.00 50.14 | | 0 |
| | MOTA | 11646 | C | SER B 357 | | 22.591 | 58.706 | 42.805 | 1.00 44.92 | | С |
| | MOTA | 11647 | Ö | SER B 357 | | 22.032 | 57.767 | 43.335 | 1.00 49.30 | | 0 |
| | ATOM | 11648 | N | ALA B 358 | | 22.822 | 59.824 | 43.458 | 1.00 47.90 | | N |
| 25 | MOTA | 11650 | CA | ALA B 358 | | 22.455 | 59.955 | 44.856 | 1.00 50.90 | | C |
| 35 | MOTA | 11652 | CB | ALA B 358 | | 22.871 | 61.301 | 45.346 | 1.00 52.95 | . , | C |
| | MOTA | 11656 | С | ALA B 358 | | 20.962 | 59.764 | 45.155 | 1.00 51.41 | | C, |
| | ATOM | * | 0. | ALA B 358 | | 20.538 | 59.955 | 46.293 | 1.00 50.45 | | 0 |
| | MOTA | 11657 | | CYS B 359 | | 20.158 | 59.408 | 44.167 | 1.00 51.99 | | N |
| 40 | MOTA | 11658 11660 | N CA | CYS B 359 | | 18.739 | 59.237 | 44.444 | 1.00 56.13 | | ·C |
| 40 | ATOM | | | CYS B 359 | | 17.928 | 60.518 | 44.118 | 1.00 57.03 | | С |
| | ATOM | 11662 | CB SG | CYS B 359 | | 17.612 | 60.710 | 42.327 | 1.00 70.47 | | S |
| ٠ | ATOM | 11665 | C | CYS B 359 | | 18.122 | | 43.726 | 1.00 51.20 | | С |
| | ATOM | 11666 | | CYS B 359 | | 16.907 | 58.001 | | 1.00 57.81 | | 0 |
| 4.5 | ATOM | | | HIS B 360 | | 18.909 | 57.107 | 43.238 | 1.00 46.00 | | N |
| 45 | ATOM | 11668 | N | | | 18.286 | • | 42.602 | 1.00 46.33 | | C |
| | MOTA | | | | | 19.256 | | 41.736 | 1.00 43.36 | | С |
| | MOTA | | CB | HIS B 360 | | 20.215 | | | 1.00 38.68 | | С |
| | ATOM | | .CG | HIS B 360 | | | | | | | N |
| | MOTA | | ND | 1 HIS B 360 | | 21.398 | | | | | C |
| 50 | ATOM | 11678 | CE | 1 HIS B 360 | | 22.052 | | | | | N |
| | ATOM | | | 2 HIS B 360 | | 21.334 | | | | | C |
| | MOTA | 11682 | CD | 2 HIS B 360 | | 20.178 | | | | | Č |
| | MOTA | 11684 | C | HIS B 360 | | 17.608 | _ | | | | ō |
| | ATOM | 11685 | 0 | HIS B 360 | | 18.049 | | | | | N |
| 55 | ATOM | 11686 | N | VAL B 361 | | 16.521 | | | | • | C |
| • | ATOM | | | | | 15.712 | | | | | C |
| | ATOM | | CE | | | 14.359 | | | | | C |
| | ATOM | | . CG | 1 VAL B 361 | | 13.659 | 52.119 | | | | C |
| | ATOM | | • | 2 VAL B 361 | | 13.474 | | | | | |
| 60 | ATOM | | | VAL B 361 | | 16.427 | | | | | С |
| | ATOM | | | VAL B 361 | | 16.805 | 51.659 | 43.055 | 1.00 50.03 | • | . 0 |
| | | | | | | | | | | | |

| | | | | · · | | | | | | | 3.7 |
|-----|--------|-----------|-----|-------------|----------|--------|--------|------------|-----|----|-----|
| 5 | ATOM | 11702 | N | HIS B 362 | 16.636 | 51.656 | 45.235 | 1.00 50.40 | | | N |
| | | 11704 | | HIS B 362 | 17.322 | 50.373 | 45.323 | 1.00 54.92 | | | С |
| | ATOM | | | | 18.864 | 50.539 | 45.254 | 1.00 54.49 | | | C |
| | MOTA | 11706 | | HIS B 362 | | | 46.321 | 1.00 60.33 | | | С |
| | ATOM | 11709 | | HIS B 362 | 19.377 | 51.443 | | 1.00 66.26 | | | N |
| | ATOM | 11710 | | HIS B 362 | 19.017 | 52.771 | 46.390 | | | | |
| 10 | ATOM : | 11712 | CE1 | HIS B 362 | 19.596 | 53.328 | 47.442 | 1.00 65.09 | | | С |
| 1.0 | ATOM | 11714 | | HIS B 362 | 20.305 | 52.406 | 48.065 | 1.00 61.43 | | | N |
| | | 11716 | | HIS B 362 | 20.174 | 51.216 | 47.389 | 1.00 61.57 | | | С |
| | MOTA | | | HIS B 362 | 16.929 | 49.742 | 46.671 | 1.00 54.45 | | | С |
| | ATOM | 11718 | С | | | 50.242 | 47.362 | 1.00 53.82 | | ٠. | 0 |
| | MOTA | 11719 | О | HIS B 362 | 16.069 | | 47.059 | 1.00 53.43 | | | N |
| 15 | ATOM | 11720 | N | ASP B 363 | 17.564 | 48.650 | | 1.00 54.67 | • | | C |
| | ATOM | 11722 | CA | ASP B 363 | 17.217 | 48.054 | 48.320 | | | | c |
| | ATOM | 11724 | CB | ASP B 363 | 16.494 | 46.752 | 48.043 | 1.00 56.65 | | | |
| | MOTA | 11727 | CG | ASP B 363 | 17.334 | 45.830 | 47.255 | 1.00 56.00 | | | C, |
| • | MOTA | 11728 | | ASP B 363 | 18.346 | 45.373 | 47.833 | 1.00 60.63 | | | 0 |
| 20 | | | | ASP B 363 | 17.083 | 45.532 | 46.063 | 1.00 51.94 | | | 0 |
| 20 | MOTA | | | | 18.443 | 47.756 | 49.171 | 1.00 55.74 | | | С |
| | ATOM | 11730 | С | ASP B 363 | | | | 1.00 54.34 | | | 0 |
| | MOTA | 11731 | 0 | ASP B 363 | 19.562 | 48.178 | 48.890 | 1.00 54.75 | | | N |
| | ATOM | 11732 | N | GLU B 364 | 18.180 | 46.998 | 50.216 | | | | C |
| | ATOM | 11734 | CA | GLU B 364 | 19.153 | 46.627 | 51.197 | 1.00 58.19 | | | |
| 25 | ATOM | 11736 | СВ | GLU B 364 | 18.486 | 45.696 | 52.252 | 1.00 66.95 | | | С |
| 2.7 | | 11739 | CG | GLU B 364 | 17.379 | 44.737 | 51.746 | 1.00 73.62 | - | | С |
| | ATOM | | | GLU B 364 | 15.939 | 45.284 | 51.760 | 1.00 79.77 | | | C |
| | MOTA | 11742 | | | 15.620 | 46.193 | 50.945 | 1.00 81.19 | | | 0 |
| | MOTA | 11743 | | GLU B 364 | | | 52.581 | 1.00 79.52 | | | 0 |
| | ATOM | 11744 | OE2 | GLU B 364 | 15.110 | 44.780 | | 1.00 53.23 | | | Č |
| 30 | ATOM | 11745 | С | GLU B 364 | 20.436 | 46.015 | 50.655 | | | | Ö |
| | MOTA | 11746 | 0 | GLU B 364 | 21.497 | 46.365 | 51.142 | 1.00 62.76 | | | |
| | ATOM | 11747 | N | PHE B 365 | 20.359 | 45.146 | 49.652 | 1.00 48.86 | | | N |
| | ATOM | 11749 | CA | PHE B 365 | 21.509 | 44.351 | 49.213 | 1.00 45.25 | | | С |
| | | | СВ | PHE B 365 | 21.180 | 42.866 | 49.376 | 1.00 47.71 | | | С |
| 26 | MOTA | 11751 | | | 20.355 | 42.527 | | 1.00 47.10 | | | С |
| 35 | MOTA | 11754 | CG | PHE B 365 | | 42.462 | 50.470 | 1.00 48.77 | | | C |
| | ATOM | 11755 | | PHE B 365 | 19.002 | | 51.573 | 1.00 50.48 | | | Ċ |
| | ATOM | 11757 | | PHE B 365 | | 42.134 | | | | | ,C |
| | ATOM | 11759 | CZ | PHE B 365 | 18.807 | 41.860 | 52.769 | 1.00 50.39 | | | Ċ |
| | MOTA | 11761 | CE2 | PHE B 365 | 20.163 | 41.906 | 52.892 | 1.00 49.25 | | | - |
| 40 | ATOM | 11763 | CD2 | PHE B 365 | 20.941 | 42.236 | 51.784 | 1.00 52.57 | | | С |
| , , | MOTA | 11765 | С | PHE B 365 | 22.028 | 44.401 | 47.758 | 1.00 48.01 | | | C |
| | | 11766 | ō | PHE B 365 | | 43.488 | 47.355 | 1.00 48.65 | | | 0 |
| | ATOM. | | | ARG B 366 | | 45.387 | 46.959 | 1.00 41.71 | | | N |
| | MOTA | 11767 | N. | | | 45.495 | 45.595 | 1.00 38.21 | | | C |
| | MOTA | 11769 | CA | | | | | 1.00 44.13 | • | | C |
| 45 | MOTA | 11771 | | ARG B 366 | | 44.800 | 44.631 | | | | č |
| | ATOM | ··· 11774 | CG | ARG B 366 | | 43.373 | 44.547 | 1.00 45.53 | | | c |
| | ATOM | 11777 | CD | ARG B 366 | 21.069 | 42.891 | 43.182 | 1.00 47.33 | | | |
| | ATOM | | NE | ARG B 366 | 19.640 | 42.980 | 42.943 | 1.00 46.43 | | | N |
| : | ATOM | 11782 | CZ | ARG B 366 | | 42.079 | 42.253 | 1.00 48.01 | | • | С |
| 50 | | | | ARG B 366 | | | 41.765 | 1.00 42.06 | • • | • | . N |
| 50 | ATOM | | | | | | 42.048 | | | | N |
| • | MOTA | | | 2 ARG B 366 | | | | | | | С |
| | MOTA | 11789 | С | ARG B 366 | | | 45.262 | | | | ŏ |
| | ATOM | 11790 | 0 | ARG B 366 | | | 45.778 | | | | |
| | ATOM | | N | THR B 367 | 22.812 | | 44.353 | | | | N |
| 55 | ATOM | | | THR B 367 | | 48.806 | 44.093 | | | | ,C |
| 55 | Y WUM | 11795 | | THR B 367 | | | 45.030 | | | | С |
| | | | CD. | | | | | · | | | 0 |
| | ATOM | | | L THR B 367 | | | | | | | С |
| | ATOM | | | | | | | | | | c |
| | MOTA | | | THR B 367 | | | | | | • | ő |
| 60 | ATOM | 11804 | 0 | THR B 367 | | | | | | | |
| • | ATOM | | N | ALA B 368 | 3 22.734 | 50.097 | 42.088 | 1.00 49.08 | | | N |
| | | | | | | | | | | | |

```
23.096 50.539
22.408 51.789
24.589 50.768
                                          23.096 50.539
                                                            40.742
                                                                     1.00 46.61
                        ALA B 368
            11807
                    CA
     MOTA
                                                                      1.00 48.60
                                                            40.479
                        ALA B 368
                    CB
           11809
     MOTA
                                                                      1.00 47.51
                                                                                              C
                                                            40.715
                    С
                        ALA B 368
     ATOM 11813
                                       25.131
                                                   51.084
                                                            41.752
                                                                      1.00 54.43
                        ALA B 368
     ATOM 11814
                    0
                                                                      1.00 46.20
                                        25.248
                                                   50.662
                                                            39.561
                        ALA B 369
     MOTA
            11815
                                                                      1.00 45.00
                                                            39.528
                                                   50.690
                        ALA B 369
                                         26.685
            11817
10 ATOM
                                                                      1.00 47.24
                                                   49.328
                                                            40.018
                                          27.158
                        ALA B 369
            11819
                    CB
     ATOM
                                                  51.050
                                                            38.249
                                                                      1.00 44.87
                                          27.496
                         ALA B 369
            11823
                    С
     MOTA
                                                                                            . 0
                                                                      1.00 48.30
                                                  50.643
                                                            37.116
                         ALA B 369
                                          27.161
            11824
                    0
     MOTA
                                                                                              N
                                                                      1.00 42.20
                                                   51.759
                                                            38.447
                         VAL B 370
                                          28.620
            11825
                    N
     MOTA
                                                                                              C
                                                                      1.00 38.93
                                                   52.125
                                                            37.315
                                          29.468
     MOTA
            11827
                    CA
                         VAL B 370
15
                                                                                              С
                                                                      1.00 36.63
                                                   53.628
                                                            37.014
                                          29.495
                         VAL B 370
     ATOM
            11829
                    CB
                                                                                              C
                                                                      1.00 41.13
                                                   53.873
                                                            35.921
                                          30.429
                    CG1 VAL B 370
     MOTA
            11831
                                                                                              C
                                                                      1.00 37.20
                                                  54.161
                                                            36.602
                                          28.134
                   AL B

VAL B 3.

GLU B 371

GLU B 371

GLU B 371

GEU B 371

CD GLU B 371

OE1 GLU B 371

OE2 GLU B 371

GLU B 372

GLU B 372

32.935

49.5

GLY B 372

34.842

50.165

Y B 372

37.272

49.955

37.272

38.339

49.86

38.364

49.5

39.716

50.7

40.533

49

3.682

50

91

4
                    .CG2 VAL B 370
            11835
     ATOM
                                                                      1.00 38.61
                                                            37.636
                                          30.838
                                                   51.685
                         VAL B 370
            11839
     MOTA
                                                                                              0
                                                            38.525
                                                                      1.00 38.62
20
     MOTA
            11840
                                                                      1.00 43.13
                                                                                              N
                                                            36.885
    ATOM
            11841
                                                                                              Ċ
                                                                      1.00 41.26
                                                            37.276
            11843
     MOTA
                                                                                              С
                                                             37.822
                                                                      1.00 43.99
     ATOM
            11845
                                                                                              С
                                                             39.157
                                                                      1.00 46.24
            11848
     MOTA
                                                                                              С
                                                             39.677
                                                                      1.00 51.18
            11851
25
     MOTA
                                                                      1.00 54.14
                                                             40.880
     MOTA
            11852
                                                                      1.00 53.22
                                                             38.927
     ATOM
            11853
                                                                      1.00 43.69
                                                             36.085
     MOTA
            11854
                                                             35.040
                                                                      1.00 40.57
            11855
     MOTA
                                                                                              N
                                                             36.240
                                                                      1.00 49.03
30 ATOM
            11856
                                                                                               C
                                                             35.201
                                                                      1.00 46.30
     ATOM
            11858
                                                                                               С
                                                                      1.00 47.83
                                                             35.731
     MOTA
             11861
                                                                      1.00 53.24
                                                             36.939
             11862
      ATOM
                                                                      1.00 48.85
                                                                                              N
                                                             34.922
      MOTA
             11863
                                                   49.535 - 33.488
                                                                                               C
                                                                      1.00 47.06
            11864
35
     MOTA
                                                                      1.00 44.96
                                                             33.023
            11866
     MOTA
                                                                                               C
                                                             34.115
                                                                      1.00 43.41
      MOTA
            11869
                                                                      1.00 43.08 --
                                                             35.387
            11872
      ATOM
                                                                      1.00 50.22
                                                             33.219
      MOTA
            11875
                                                                      1.00 57.42
                                                             33.964
                                                    47.394
                          PRO B 373
                                           39.130
    ATOM
            11876
                     0
                                                                      1.00 51.76
                                                             32.137
                                           37.903
                                                    47.658
                          PHE B 374
             11877
                     N
      MOTA
                                                                                               C
                                                             31.713
                                                                      1.00 53.93
                                                    46.319
                                           38.030
                          PHE B 374
             11879
                     CA
      MOTA
                                                             31.494
                                                                      1.00 56.43
                                                                                               C
                                           36.648
                                                    45.693
                          PHE B 374
      MOTA
             11881
                     CB
                                                                      1.00 53.63
                          PHE B 374
                                           35.736
                                                    45.873
                                                             32.661
             11884
                     CG
      MOTA
                                       35.069
                                                                      1.00 54.53
                                                             32.842
                     CD1 PHE B 374
                                                    47.063
45
      MOTA
             11885
                                       34.249
34.093
34.758
35.572
38.736
38.433
39.692
                                                             33.904
                                                                       1.00 56.48
                     CE1 PHE B 374
                                                    47.242
             11887
      MOTA
                                                                       1.00 57.87
                                                    46.226
                                                             34.821
                          PHE B 374
             11889
                     CZ
      MOTA
                                                             34.654
                                                                       1.00 50.55
                                           34.758 45.038
             11891
                     CE2 PHE B 374
      MOTA
                                                             33.579
                                                                       1.00 49.47
                                           35.572 44.865
                     CD2 PHE B 374
             11893
      MOTA
                                                             30.420
                                                                       1.00 59.86
                                                    46.536
50 ATOM
                          PHE B 374
             11895
                     Ċ
                          PHE B 374
                                                    47.466
                                                             29.694
                                                                       1.00 62.61
             11896
                     0
      ATOM
                                                             30.129
                                                                       1.00 68.35
                          VAL B 375
                                           39.692
                                                   45.677
      ATOM
             11897
                     N
                                                             28.857
                                                                       1.00 68.00
                          VAL B 375
                                           40.369
                                                    45.737
             11899
                     CA
    MOTA
                                                             28.921
                                                                       1.00 69.56
                                           41.765
                                                    45.125
                          VAL B 375
             11901
                     CB
      MOTA
                                                             27.585
                                                                       1.00 72.03
                                           42.126
                                                    44.497
                     CG1 VAL B 375
55
             11903
      MOTA
                                                                                               C
                                                              29.334
                                                                       1.00 71.07
                                           42.774
                                                     46.194
                     CG2 VAL B 375
      ATOM
             11907
                                                    45.050
                                                             27.808
                                                                       1.00 72.55
                          VAL B 375
                                           39.508
      MOTA
             11911
                     С
                                                              27.984
                                                                       1.00 64.78
                          VAL B 375
                                           39.061
                                                    43.915
             11912
                     0
      MOTA
                                                              26.712
                                                                       1.00 81.41
                          THR B 376
                                           39.275
                                                   45.774°
      MOTA
             11913
                     N
                                                    45.296
                                                             25.589
                                                                       1.00 86.08
                          THR B 376
                                           38.464
 60
             11915
                     CA
      ATOM
                                                    45.981
                                                             25.640
                                                                       1.00 85.71
                                           37.142
                          THR B 376
     ATOM 11917
                     CB
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| | | | | | | | | | | 1 00 00 06 | • | | ^ |
|-----|--------------|----------------|---------|-------|-------|---|--------|--------|----------|------------|-----|---|----|
| 5 | ATOM | 11919 | OG1 | THR B | 376 | | 36.993 | 46.575 | 26.932 | 1.00 88.06 | | | 0 |
| • | ATOM | 11921 | CG2 | THR B | 376 | • | 35.986 | 44.970 | 25.508 | 1.00 86.58 | | | C |
| | ATOM | 11925 | С | THR B | 376 | | 39.130 | 45.590 | 24.246 | 1.00 90.80 | | | С |
| | ATOM | 11926 | 0 | THR B | 376 | | 39.889 | 46.565 | 24.111 | 1.00 93.52 | | | 0 |
| | ATOM | 11927 | | LEU E | 377 | | 38.840 | 44,768 | 23.240 | 1.00 94.98 | | | N |
| 10 | ATOM | 11929 | CA | LEU E | | | 39.572 | 44.884 | 21.974 | 1.00 97.54 | | | С |
| 10 | ATOM | 11931 | CB | LEU E | | | 40.491 | 43.667 | 21.839 | 1.00 97.95 | | | С |
| | ATOM | 11934 | CG | LEU E | | | 41.234 | 43.239 | 23.119 | 1.00 97.10 | | | С |
| | ATOM | 11936 | | LEU E | | | 42.302 | 42.213 | 22.767 | 1.00 96.01 | | | С |
| | ATOM | 11940 | | LEU E | | | 41.873 | 44.413 | 23.852 | 1.00 96.18 | | | С |
| 15 | ATOM | 11944 | C | | 3 377 | | 38.777 | 45.053 | 20.662 | 1.00 98.30 | | | ,C |
| 13 | ATOM | 11945 | Ö, | LEU I | | | 37.719 | 44.425 | 20.470 | 1.00 95.52 | | | 0 |
| | MOTA | 11946 | N. | ASP I | | | 39.328 | 45.909 | 19.782 | 1.00 97.57 | | | N |
| | | 11948 | CA | ASP I | | | 38.846 | 46.107 | 18.405 | 1.00 98.72 | | | С |
| - | ATOM | 11950 | CB | ASP I | | | 38.818 | 44.778 | 17.631 | 1.00101.77 | | | С |
| 20 | MOTA | 11953 | CG | | 3 378 | | 40.161 | 44.040 | 17.668 | 1.00106.54 | | | С |
| 20 | MOTA | 11954 | | ASP I | | | 40.185 | 42.823 | 17.348 | 1.00107.57 | | | 0 |
| | ATOM | 11955 | | ASP I | | | 41.238 | 44.594 | 18.001 | 1.00108.22 | | | 0 |
| | ATOM | | C | | B 378 | | 37.466 | 46.678 | 18.517 | 1.00 95.34 | | | С |
| | ATOM | 11956 | 0 | | B 378 | | 36.576 | 46.473 | 17.690 | 1.00 90.09 | | | 0 |
| 25 | MOTA | 11957 | N | | B 379 | | 37.315 | 47.427 | 19.584 | 1.00 92.72 | | • | N |
| 25 | MOTA | 11958 | CA | | В 379 | | 36.018 | 47.850 | 19.970 | 1.00 89.67 | | | С |
| | ATOM | 11960 | CB | | B 379 | | 36.115 | 48.778 | 21.181 | 1.00 87.84 | | | С |
| | MOTA | 11962 | CG | | B 379 | | 36.814 | 48.131 | 22.363 | 1.00 85.16 | | | С |
| | ATOM | 11965 11968 | SD | | в 379 | | 36.294 | 48.757 | 23.944 | 1.00 81.06 | | | S |
| 20 | MOTA | | CE | | B 379 | | 37.408 | 49.948 | 24.177 | 1.00 82.73 | | | С |
| 30 | MOTA | 11969 | | | B 379 | | 35.455 | 48.535 | | 1.00 88.14 | | | С |
| | MOTA | 11973 11974 | 0 | | B 379 | | 34.453 | 48.097 | 18.241 | 1.00 89.91 | | | 0 |
| | MOTA | | | | B 380 | | 36.133 | 49.590 | 18.349 | | | | N |
| | ATOM | 11975 11977 | N CA | | B 380 | | 35.555 | 50.483 | 17.361 | 1.00 89.95 | | | C |
| 25 | ATOM | 11977 | CB | | B 380 | | 36.642 | 51.168 | 16.508 | 1.00 89.88 | | | C |
| 35 | | 11982 | CG | | B 380 | | 36.336 | 52.614 | 16.072 | 1.00 90.98 | | | С |
| | MOTA | 11985 | CD | | B 380 | | 34.854 | 52.999 | 16.089 | | | | С |
| | MOTA MOTA | 11986 | | | B 380 | | 34.530 | 54.085 | 16.634 | 1.00 82.43 | | | 0 |
| | ATOM | 11987 | | | в 380 | | 34.021 | 52.227 | 15.552 | 1.00 85.64 | | | 0 |
| 40 | ATOM | 11988 | C | | B 380 | | 34.529 | 49.668 | 16.547 | 1.00 90.22 | | | С |
| 40 | MOTA | 11989 | . 0 | | B 380 | | 33.385 | 50.102 | 16.385 | 1.00 89.91 | | | О |
| | ATOM | 11990. | | | B 381 | | 34.946 | 48.482 | 16.080 | 1.00 89.23 | ŀ | | N |
| | ATOM | 11992 | CA | | B 381 | | 34.122 | 47.536 | 15.284 | 1.00 85.33 | | | С |
| | ATOM | 11994 | | | B 381 | | 34.705 | 46.142 | 15.374 | 1.00 86.39 |) | | С |
| 45 | ATOM | 11997 | CG | | B 381 | | 35.859 | 45.959 | 14.456 | 1.00 91.21 | . • | | С |
| 73 | MOTA | 11998 | | | B 381 | | 35,821 | 46.563 | 13.353 | | | | 0 |
| | MOTA | 11999 | 002 | ASP | B 381 | | 36.842 | 45.237 | 14.742 | 1.00 97.75 | , | | 0 |
| | ATOM | | | | B 381 | | 32.676 | | 15.606 | 1.00 79.23 | · · | | С |
| | MOTA | | ŏ | | B 381 | | 31.926 | | | 1.00 79.04 | ļ | | 0 |
| 50 | MOTA | | | | B 382 | | 32.270 | | | |) | | N |
| .50 | ATOM | | CA | | B 382 | | 30.891 | | | | 3 | | С |
| | ATOM | | | | B 382 | | 30.801 | | - 18.685 | | 3 | | С |
| | ATOM | | | | B 382 | | 32.081 | | | | 3 | | S |
| ٠. | ATÓM | | | | B 382 | | 30.101 | | | | . • | | С |
| 55 | | | | | B 382 | | 28,891 | | | • | 7 | | 0 |
| رر | ATOM | | | | B 383 | | 30.838 | | | | 5 | | N |
| • | ATOM | | | | B 383 | | 30.295 | | | | 3 | | С |
| | ATOM ATOM | | | | B 383 | | 29.732 | | | | | | С |
| | ATOM | | | | B 383 | | 30.294 | | | | 5 | | 0 |
| 60 | • | | | | B 384 | | 28.597 | | | | | | N |
| UU | ATOM | | | | B 384 | | 27.915 | | | | | | С |
| | ATOM | 12021 | , UA | IIV | P 204 | | _,, | 22 | | | | | |

| | | | • | | | | • | | | • | | | | |
|-----|------|-------|-------|-------|-----|---|--------|--------|--------|---------|-------|---|---|---------|
| 5 | ATOM | 12023 | CB T | YR B | 384 | | 26.468 | 50.421 | 13.020 | 1.00 63 | | | | С |
| , | ATOM | 12026 | | YR B | | | 25.620 | 50.091 | 11.867 | 1.00 5 | | | | С |
| | ATOM | 12027 | CD1 T | | | | 25.280 | 48.777 | 11.578 | 1.00 5 | 9.47 | | | С |
| | ATOM | 12029 | CE1 T | | | | 24.476 | 48.469 | 10.515 | 1.00 6 | 1.28 | | | С |
| ٠ | | 12023 | | YR B | | | 23.997 | 49.497 | 9.733 | 1.00 6 | 2.97 | | | С |
| 10 | MOTA | | | YR B | | | 23.179 | 49.288 | 8.636 | 1.00 6 | | | | 0 |
| 10 | ATOM | 12032 | | | | | 24.332 | 50.792 | 10.028 | 1.00 6 | | | | С |
| | MOTA | 12034 | CE2 T | | | | | 51.079 | 11.083 | 1.00 6 | | | | С |
| | MOTA | 12036 | CD2 T | | | | 25.136 | | 11.732 | 1.00 6 | | | | Č |
| | MOTA | 12038 | | YR B | | | 28.185 | 51.536 | | 1.00 6 | | | | ō |
| | MOTA | 12039 | | YR B | | | 28.365 | 52.708 | 12.106 | | | | | N |
| 15 | ATOM | 12040 | | SN B | | | 28.213 | 51.178 | 10.464 | 1.00 7 | | | | |
| | ATOM | 12042 | | SN B | | | 28.501 | 52.166 | 9.438 | 1.00 7 | | | | C |
| | ATOM | 12044 | CB A | SN B | 385 | | 29.894 | 51.890 | 8.828 | 1.00 7 | | • | | С |
| | ATOM | 12047 | CG A | SN B | 385 | | 31.057 | 51.931 | 9.889 | 1.00 7 | | | | С |
| _ | ATOM | 12048 | OD1 A | SN B | 385 | | 30.989 | 52.640 | 10.887 | 1.00 8 | | - | | 0 |
| 20 | ATOM | 12049 | ND2 A | | | | 32.111 | 51.163 | 9.646 | 1.00 7 | | | | N |
| 20 | ATOM | 12052 | | SN B | | | 27.362 | 52.205 | 8.374 | 1.00 7 | | | | С |
| | ATOM | 12053 | | | 385 | | 27.234 | 51.384 | 7.455 | 1.00 7 | 9.49 | | | 0 |
| | | 12054 | OXTA | | | | 26.445 | 53.064 | 8.344 | 1.00 7 | 9.45 | | | 0 - |
| | MOTA | | | SER C | -2 | | 53.798 | 42.195 | 56.398 | 1.00 5 | | | | N |
| 0.5 | ATOM | 12055 | | SER C | -2 | - | 54.991 | 42.203 | 57.314 | 1.00 5 | | | | С |
| 25 | MOTA | 12057 | | | | | 54.496 | 42.894 | 58.620 | 1.00 5 | | | | С |
| | ATOM | 12059 | | SER C | | | | 43.571 | 58.434 | 1.00 5 | | | | 0 |
| | MOTA | 12062 | | SER C | | | 53.217 | | 57.607 | 1.00 5 | | | | Ċ |
| | MOTA | 12064 | | SER C | | | 55.846 | 40.853 | | 1.00 5 | | | | ŏ |
| | MOTA | 12065 | | SER C | | | 56.969 | 40.946 | 58.008 | 1.00 4 | | | | N |
| 30 | MOTA | 12068 | | PHE C | | | 55.366 | 39.626 | 57.416 | | | | | C |
| | ATOM | 12070 | CA I | PHE C | | | 56.183 | 38.439 | 57.772 | 1.00 4 | | | | C |
| | ATOM | 12072 | CB I | PHE C | -1 | | 55.401 | 37.604 | 58.777 | 1.00 4 | | | | |
| | ATOM | 12075 | CG I | PHE C | -1 | | 54.686 | 38.446 | 59.773 | 1.00 4 | | | | C |
| | ATOM | 12076 | CD1 I | PHE C | -1 | | 53.717 | 39.362 | 59.347 | 1.00 3 | | | | C |
| 35 | MOTA | 12078 | CE1 | PHE C | -1 | | 53.068 | 40.151 | 60.248 | 1.00 4 | | | | С |
| | ATOM | 12080 | CZ I | PHE C | -1 | | 53.371 | 40.058 | 61.605 | 1.00 3 | | | | С |
| • | ATOM | 12082 | | PHE C | | | 54.336 | 39.149 | 62.031 | 1.00 4 | 15.60 | | | С |
| | ATOM | 12084 | CD2 | PHE C | -1 | | 54.990 | 38.355 | 61.111 | | | | | С |
| | ATOM | 12086 | | PHE C | | | 56.784 | 37.524 | 56.676 | 1.00 4 | | | | С |
| 40 | ATOM | 12087 | | PHE C | | | 56.404 | 36.379 | 56.469 | 1.00 4 | 18.73 | - | | 0 |
| 40 | ATOM | 12088 | | VAL C | | | 57.769 | 38.075 | 56.011 | 1.00 | 16.82 | | | N |
| | ATOM | 12090 | | VAL C | | | 58.543 | 37.462 | 54.968 | 1.00 | 12.56 | | | С |
| | ATOM | 12092 | | VAL C | | • | 59.695 | 38.359 | 54.783 | 1.00 | 48.99 | | | С |
| • | ATOM | 12094 | | VAL C | | | 59.357 | 39.397 | 53.764 | 1.00 | 51.10 | | | С |
| 15 | | | | VAL C | | | 60.001 | 39.049 | 56.107 | 1.00 | | | | С |
| 45 | MOTA | 12098 | | | | | 59.140 | 36.107 | 55.089 | 1.00 | | | | C |
| | MOTA | 12102 | | VAL C | | | 59.300 | 35.444 | 54.090 | 1.00 | | | | . C . O |
| | ATOM | 12103 | | VAL C | | | | 35.666 | 56.275 | 1.00 | | | | N |
| | ATOM | 12104 | | GLU (| | | 59.520 | 34.310 | 56.418 | 1.00 | | | | С |
| ~~ | MOTA | 12106 | | GLU (| | | 60.053 | | 57.864 | 1.00 | | | | Č |
| 50 | ATOM | 12108 | | GLU (| | | 60.580 | 34.062 | | | | | | Č |
| | MOTA | 12111 | | GLU (| | | 61.892 | 33.262 | 57.999 | 1.00 | | | | č |
| | MOTA | | | GLU (| | | 61.893 | 32.085 | 59.020 | | | | | o |
| | MOTA | 12115 | | GLU (| | | 61.939 | 32.255 | 60.267 | 1.00 | | | | |
| | MOTA | 12116 | | GLU (| | | 61.884 | 30.928 | 58.557 | | | | • | . 0 |
| 55 | ATOM | 12117 | C | GLU (| 2 1 | | 58.883 | 33.376 | | | | | | Ċ |
| | ATOM | | | GLU (| C 1 | | 59.026 | | | | | | | 0 |
| | ATOM | | | MET (| | | 57.696 | | 56.493 | • | | | | N |
| • | ATOM | | | MET (| | | 56.532 | | | | | | | С |
| | ATOM | | | MET (| | | 55.626 | 33.430 | | | | | | С |
| 60 | ATOM | | | MET (| | | 56.231 | 33.224 | 59.038 | 1.00 | 45.70 | | | С |
| 00 | ATOM | | | MET | | | 55.044 | | | 1.00 | 51.30 | | | S |
| | VION | 1010 | ~~ | | | | | | | | | | | |

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60.885
                                                              1.00 55.15
                                              34.710
                                      54.993
          12130
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                        LYS C
      MOTA
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|------|------|-------|-----|-------|-----|----|---|--------|--------|--------|------|---------|---|---|-----|
| 5 | MOTA | 12249 | 0 | LYS 4 | С | 9 | | 44.734 | 20.619 | 49.076 | | 66.42 | | | 0 |
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| | MOTA | 12252 | CA | SER | С | 10 | | 42.295 | 21.547 | 48.244 | | 56.42 | | | С |
| | ATOM | 12254 | CB | SER | | 10 | | 41.188 | 22.179 | 47.413 | | 58.97 | | | С |
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| 10 | MOTA | 12259 | c | SER | | 10 | | 42.115 | 20.024 | 48.308 | 1.00 | 59.45 | | | С |
| 10 | | 12260 | ō | SER | | 10 | | 41.760 | 19.470 | 49.366 | 1.00 | 61.04 | | | 0 |
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| • | ATOM | 12263 | CA | | | 11 | | 42.837 | 17.013 | | | 50.69 | | | С |
| | MOTA | 12266 | C | GLY | | | | 42.155 | 16.131 | 48.456 | | 47.76 | • | | 0 |
| 15 | MOTA | 12267 | 0 | GLY | | 11 | | | | 48.304 | | 51.44 | | | N |
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| | MOTA | 12270 | CA | GLN | | 12 | | 44.796 | 16.397 | 49.296 | | 51.49 | | | č |
| | ATOM | 12272 | CB | GLN | | 12 | • | 45.904 | 15.638 | 48.615 | | | | | C |
| | MOTA | 12275 | CG | GLN | С | 12 | | 45.346 | 15.061 | 47.327 | | 57.41 | | | C |
| 20 | ATOM | 12278 | CD | GLN | C, | 12 | | 46.330 | 14.266 | 46.496 | | 62.60 | | | |
| | MOTA | 12279 | OE1 | GLN | С | 12 | | 47.536 | 14.564 | 46.471 | | 67.40 | • | | 0 |
| | ATOM | 12280 | NE2 | GLN | С | 12 | | 45.816 | 13.255 | 45.798 | | 64.74 | | | N |
| | ATOM | 12283 | С | GLN | С | 12 | | 45.284 | 17.244 | 50.466 | | 51.33 | | | C |
| | ATOM | | 0 | GLN | | 12 | | 45.770 | 16.759 | 51.487 | | 53.08 | | | O. |
| 25 | ATOM | 12285 | N | GLY | | 13 | | 45.147 | 18.538 | 50.320 | | 50.28 | | | N |
| 23 | ATOM | 12287 | CA | GLY | | 13 | | 45.357 | 19.400 | 51.455 | 1.00 | 48.93 | | | С |
| | ATOM | 12290 | C | GLY | | 13 | | 46.550 | 20.283 | 51.408 | 1.00 | 42.27 | | | С |
| | | | ŏ | GLY | | 13 | | 47.417 | 20.135 | 50.579 | 1.00 | 38.82 | | | 0 |
| | ATOM | 12291 | | TYR | | 14 | | 46.581 | 21.229 | 52.329 | | 44.75 | - | | N |
| 20 | ATOM | 12292 | И | | | 14 | | 47.763 | 22.054 | 52.493 | | 42.35 | | | С |
| 30 | ATOM | 12294 | CA | TYR | | 14 | | 47.703 | 23.465 | 52.768 | | 39.78 | | | С |
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| | ATOM | 12299 | CG | TYR | | 14 | | 46.558 | | 51.430 | | 41.19 | | | Ċ |
| | MOTA | 12300 | | TYR | | 14 | | 45.196 | 23.694 | 50.330 | | 37.98 | | | . č |
| | MOTA | 12302 | | TYR | | 14 | | 44.482 | 24.133 | | | 51.75 | | | č |
| 35 | ATOM | 12304 | CZ | TYR | | 14 | | 45.138 | 24.850 | 49.355 | | 60.99 | | | ő |
| | MOTA | 12305 | ОН | TYR | | 14 | | 44.440 | 25.307 | 48.237 | | | | | c |
| | MOTA | 12307 | | TYR | | 14 | | 46.508 | 25.122 | 49.486 | | 48.63 | | | c |
| | ATOM | 12309 | CD2 | TYR | | 14 | | 47.201 | 24.665 | 50.587 | | 36.78 | | | c |
| | MOTA | 12311 | С | TYR | | 14 | | 48.582 | 21.534 | 53.621 | | 42.85 | | | 0 |
| 40 | MOTA | 12312 | . 0 | TYR | | 14 | | 48.031 | 21.156 | 54.661 | | 46.82 | | | |
| | ATOM | 12313 | N | TYR | | 15 | | 49.901 | 21.495 | 53.419 | | 47.44 | | • | N |
| | ATOM | 12315 | CA | TYR | С | 15 | | 50.864 | 21.109 | 54.484 | | 40.77 | | | C |
| | ATOM | 12317 | CB | TYR | C | 15 | | 51.541 | 19.780 | 54.155 | | 39.30 | | | C |
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| 45 | ATOM | 12321 | CD1 | TYR | С | 15 | | 53.646 | 19.867 | 52.722 | | 36.76 | | | C |
| | ATOM | 12323 | CE1 | TYR | C | 15 | | 54.335 | 19.731 | 51.545 | | 33,20 | | | С |
| • | ATOM | 12325 | | TYR | | 15 | • | 53.703 | 19.360 | 50.429 | 1.90 | 37.91 | | | С |
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| | | | | TYR | | 15 | | 52.453 | | 53.816 | 1.00 | 40.28 | | | 0 |
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| 55 | ATOM | | | VAL | | 16 | | 53.114 | | | | 40.96 | | | c |
| • | ATOM | | | VAL | | 16 | | | | | | 7 40.50 | | | č |
| | ATOM | | | 2 VAL | | 16 | | 54.458 | | | | 37.23 | | | č |
| | ATOM | | | VAI | | | | 54.633 | | | | | | | ō |
| ~- | ATOM | | | VAI | | | | 54.372 | | | | 0 40.88 | | | Ŋ |
| 60 | ATOM | | | GLU | | | | 55.867 | | | | 35.29 | | | C |
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                                               16.240
                                                        69.813
40
            12423
                   CB
                       SER C
                               22
      MOTA
                                                                                       0
                                       65.736
                                                        70.428
                                                                 1.00 51.42
                                               16.738
                       SER C
                               22
      MOTA
            12426
                   OG
                                                                                       C
                                                                 1.00 47.58
                                       67.639
                                               14.580
                                                        68.113
                       SER C
                               22
            12428
                   С
      ATOM
                                                                 1.00 57.41
                        SER C
                                       67.657
                                                13.570
                                                        68.805
                               22
      MOTA
            12429
                   0
                                                                 1.00 43.72
                                                        67.076
                                       68.450
                                                14.740
                        PRO C
                               23
      MOTA
            12430
                   N
                                                                 1.00 46.60
                                                                                       С
                                       68.345
                                                15.844
                                                        66.127
45
                   CA
                        PRO C
                               23
            12431
      MOTA
                                                                                       C
                                                                 1.00 44.76
                                       69.475
                                                15.527
                                                        65.140
                        PRO C
                               23
      ATOM: 12433
                   CB
                                                                                       С
                                                        65.254
                                                                1.00 41.34
                                       69.592
                                                14.109
      ATOM 12436
                   CG
                        PRO C
                               23
                                                                                       C
                                                                 1.00 38.07
                                                        66.732
                                       69.568
                                                13.881
                               23
                   CD
                        PRO C
      MOTA
            12439
                                                                                       С
                                                                 1.00 44.72
                                       67.003
                                                15.754
                                                        65.433
            12442
                   С
                        PRO C
                               23
      MOTA
                                                                 1.00 49.06
                                                        65.601
                                        66.338
                                                14.767
                        PRO C
                               23
 50
      ATOM
            12443
                   0
                                                        64.661
                                                                 1.00 50.13
                                       66.640
                                               16.763
                        PRO C
                               24
                   N
      MOTA
            12444
                                                                 1.00 45.48
                                                         64.016
                                                                                       ·C
                                                16.882
                        PRO C
                                     65.314
                               24
            12445
                   CA
      MOTA
                                                                                       С
                                                                 1.00 50.03
                                                18.328
                                                         63.526
                        PRO C
                               24
                                       65.324
            12447
                   CB
      ATOM-
                                                                                       C.
                                                         64.223
                                                                 1.00 50.43
                                       66.494
                                                19.014
            12450
                   CG
                        PRO C
                               24
      ATOM
                                                                                       С
                                                17.933
                                                         64.408
                                                                 1.00 46.95
                                       67.515
                        PRO C
                               24
      ATOM 12453
                    CD
 55
                                                                 1.00 47.53
                        PRO C
                                       64.902
                                                16.046
                                                         62.798
                               24
      ATOM · 12456
                   С
                                                         61.873
                                                                 1.00 48.93
                                                15.938
                        PRO C
                               24
                                        65.687
                   0
      ATOM
            12457
                                                                 1.00 50.98
                                                         62.799
                                                15.568
                                        63.661
                        GLN C
                               25
                    N
      ATOM 12458
                                                14.893
                                                         61.663
                                                                 1.00 49.33
                        GLN C
                               25
                                        63.096
      ATOM 12460
                    CA
                                                                                       С
                                                         62.149
                                                13.625
                                                                 1.00 53.14
                        GLN C
                               25
                                        62.395
            12462
                    CB
 60
      MOTA
                                                         62.669
                                                                 1.00 48.07
                                       63.395
                                                12.605
                        GLN C 25
      MOTA
            12465
                    CG
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| | | | | | | , | | | | | | | | | | _ |
|-------------|--------------|-------|--------|--------------|-----|-----|------------|---|--------|--------|--------|------|-------|----|---|------------|
| 5 | ATOM | 12468 | | GLN (| | 25 | | | 62.765 | 11.501 | 63.465 | 1.00 | 52.67 | | | С |
| | MOTA | 12469 | OE1 | GLN (| Ç | 25 | • | | 61.814 | 10.862 | 63.017 | | 63.47 | | | 0 |
| | ATOM | 12470 | NE2 | GLN (| С | 25 | | | 63.303 | 11.255 | 64.648 | | 46.81 | | | N |
| | MOTA | 12473 | С | GLN (| С | 25 | | | 62.148 | 15.776 | 60.845 | 1.00 | 51.50 | | | С |
| | ATOM | 12474 | 0 | GLN (| С | 25 | | | 61.039 | 16.151 | 61.274 | | 46.44 | | | 0 |
| 10 | ATOM | 12475 | N | THR | С | 26 | | | 62.595 | 16.092 | 59.643 | 1.00 | 49.81 | | | N |
| , • | ATOM | 12477 | CA | THR | С | 26 | | | 61.754 | 16.827 | 58.751 | | 51.29 | | | С |
| • | ATOM | 12479 | CB | THR | С | 26 | | | 62.462 | 17.098 | 57.429 | | 53.77 | ٠. | | C |
| | ATOM | 12481 | OG1 | THR | С | 26 | | | 63.759 | 17.659 | 57.673 | 1.00 | 53.98 | | | 0 |
| | ATOM | 12483 | CG2 | THR | C. | 26 | | | 61.709 | 18.172 | 56.629 | | 52.68 | | | С |
| 15 | ATOM | 12487 | С | THR | | 26 | | | 60.555 | 15.969 | 58.478 | | 51.30 | | | С |
| 10 | ATOM | 12488 | 0 | THR | С | 26 | ٠. | | 60.666 | 14.771 | 58.226 | | 51.90 | | | 0 |
| | ATOM | 12489 | N | LEU | | 27 | | | 59.396 | 16.594 | 58.530 | | 50.70 | | | N |
| | ATOM | 12491 | CA | LEU | | 27 | | | 58.174 | 15.933 | 58.155 | 1.00 | 43.30 | | | С |
| • | ATOM | 12493 | СВ | LEU | | 27 | <i>:</i> . | | 57.478 | 15.409 | 59.378 | | 44.64 | | | С |
| 20 | ATOM | 12496 | CG | LEU | | 27 | | | 58.218 | 14.449 | 60.281 | 1.00 | 45.47 | | | С |
| 20 | ATOM | 12498 | | LEU | | 27 | 4. | | 57.624 | 14.540 | 61.675 | | 45.75 | | | С |
| | ATOM | 12502 | | LEU | | 27 | | | 58.122 | 13.034 | 59.686 | 1.00 | 44.30 | | | С |
| | ATOM | 12506 | C | LEU | | 27 | • | | 57.323 | 17.006 | 57.577 | | 39.69 | | | С |
| | MOTA | 12507 | 0 | LEU | | 27 | | | 57.495 | 18.143 | 57.925 | 1.00 | 43.38 | | | 0 |
| .25 | ATOM | 12508 | N | ASN | | 28 | : | | 56.412 | 16.652 | 56.695 | 1.00 | 42.74 | | | N |
| .23 | ATOM | 12510 | CA | ASN | | 28 | | | 55.433 | 17.586 | 56.185 | 1.00 | 41.37 | | | С |
| | ATOM | 12510 | CB | ASN | | 28 | | | 55.194 | 17.347 | 54.703 | 1.00 | 42.25 | | | . C |
| | ATOM | 12515 | CG | ASN | | 28 | | | 56.215 | 18.014 | 53.828 | | 41.51 | | | C |
| | | 12516 | | ASN | | 28 | | | 56.417 | 17.614 | 52.679 | | 48.06 | | | 0 |
| 30 | MOTA | 12517 | | ASN | | 28 | | | 56.870 | 19.034 | 54.355 | | 48.36 | | | N |
| 30 | MOTA | 12520 | C | ASN | | 28 | | | 54.144 | 17.326 | 56.948 | | 42.07 | | | С |
| | MOTA | 12521 | o | ASN | | 28 | • | | 53.796 | 16.175 | 57.196 | | 42.00 | | | 0 |
| | ATOM | 12522 | N | ILE | | 29 | | • | 53.429 | 18.388 | | | 41.25 | | | N |
| | MOTA | 12524 | CA | ILE | | 29 | | | 52.254 | 18.282 | 58.144 | | 38.11 | | | С |
| 35 . | ATOM | 12524 | CB | ILE | | 29 | | | 52.581 | 18.909 | 59.452 | | 37.30 | | | С |
| <i>33</i> . | MOTA MOTA | 12528 | | ILE | | 29 | | | 53.888 | 18.345 | 60.002 | 1.00 | 37.82 | | | C |
| | ATOM | 12531 | | ILE | | 29 | | | 53.764 | 16.947 | 60.383 | 1.00 | 37.89 | | | Ċ |
| | ATOM | 12535 | | ILE | | 29 | | | 51.428 | 18.758 | 60.382 | 1.00 | 37.26 | | | С |
| | ATOM | 12539 | C | ILE | | 29 | | | 51.111 | 19.100 | 57.605 | 1.00 | 41.88 | | | С |
| 40 | ATOM | 12540 | ŏ | ILE | | 29 | | | 51.317 | 20.272 | 57.335 | 1.00 | 44.35 | - | | 0 |
| 70 | MOTA | 12541 | N | LEU | | 30 | | | 49.924 | 18.485 | 57.471 | 1.00 | 41.50 | | | N |
| | ATOM | 12541 | CA | LEU | | 30 | | | 48.669 | 19.159 | 57.062 | | 40.03 | | | , C |
| * | ATOM | 12545 | СВ | LEU | | 30 | | | 47.609 | 18.121 | 56.699 | 1.00 | 36.38 | | ĺ | С |
| | ATOM | 12548 | CG | LEU | | 30 | | | 46.175 | 18.515 | 56.462 | 1.00 | 43.90 | | | С |
| 45 | ATOM | 12550 | | LEU | | 30 | | | 45.650 | 17.851 | 55.272 | 1.00 | 48.94 | | | С |
| -13 | MOTA | 12554 | | LEU | | 30 | | | 45.293 | 18.120 | 57.618 | 1.00 | 49.66 | | | ·C |
| | ATOM | 12558 | C | LEU | | .30 | | | 48.071 | 20.130 | 58.085 | 1.00 | 41.43 | | | С |
| | ATOM | 12559 | ō | LEU | | 30 | | | 47.961 | | 59.261 | | 44.99 | | | 0 |
| | MOTA | 12560 | N | VAL | | 31 | | | 47.656 | 21.300 | 57.607 | 1.00 | 44.35 | | | N |
| 50 . | ATOM | 12562 | CA | VAL | | 31 | | | 47.080 | 22.312 | 58.460 | 1.00 | 40.92 | | | С |
| 50. | ATOM | 12564 | CB | | | 31 | | | 47.300 | 23.638 | 57.892 | 1.00 | 37.95 | | | С |
| | ATOM | 12566 | | VAL | | 31 | | | 46.317 | 24.595 | 58.524 | | 41.29 | | | С |
| | | | | VAL | | 31 | | | 48.718 | 24.068 | 58.132 | 1.00 | 41.26 | • | • | С |
| | MOTA | 12570 | C | VAL | | 31 | | | 45.574 | 22.155 | 58.515 | | 45.40 | | • | С |
| 55 | ATOM | 12574 | | VAL | | 31 | | | 44.885 | | 57.555 | | 46.26 | | • | 0 |
| 55 | ATOM | 12575 | O N | ASP | | | • | | 45.082 | | 59.658 | | 44.37 | | | N |
| | MOTA | 12576 | N | ASP | | | • | | 43.693 | | | | 42.08 | | | C |
| | MOTA | 12578 | CA | ASP | | | | | | 19.799 | | | 48.54 | • | | C |
| | ATOM | | CB | ASP | | | | | 42.270 | | | | 55.02 | | | С |
| <i>ς</i> Λ | MOTA | | CG | ASP 1 ASP | | | | | 41.331 | | | | 57.45 | | | 0 |
| 60 | MOTA | | | | | | | | 42.035 | | | | 54.56 | | | 0 |
| | MOTA | 12585 | ימט | 2 ASP | · · | 22 | | | 42.000 | 10.447 | | | | - | | |

| _ | * 8001 | 10506 | c | ASP C | 32 | | 42.996 | 22.030 | 60.996 | 1.00 42.96 | | • | Ç |
|----|--------|--------|--------|---------|------|---|--------|------------------|------------------|--------------------------|---|---|----|
| 5 | MOTA | 12586 | С 0 | ASP C | 32 | | 43.171 | 21.653 | 62.148 | 1.00 38.86 | | | Ó |
| | ATOM | 12587 | N | THR C | 33 | | 42.205 | 23.072 | 60.670 | 1.00 42.49 | | | N |
| | MOTA | 12588 | | THR C | 33 | | 41.382 | 23.757 | 61.655 | 1.00 34.59 | | | С |
| | MOTA | 12590 | CA | THR C | 33 | | 41.102 | 25.275 | 61.297 | 1.00 40.43 | | | C |
| •• | MOTA | 12592 | CB | | 33 | | 40.271 | 25.418 | 60.128 | 1.00 36.06 | | | 0 |
| 10 | ATOM | 12594 | _ | THR C | 33 | | 42.332 | 26.064 | 60.943 | 1.00 38.42 | | | С |
| | ATOM | 12596 | CG2 | | | | 40.025 | 23.151 | 61.903 | 1.00 37.84 | | | С |
| • | ATOM | 12600 | C | THR C | 33 | | 39.181 | 23.773 | 62.562 | 1.00 42.84 | | | 0 |
| | ATOM | 12601 | 0 | THR C | 33 | | 39.792 | 21.985 | 61.347 | 1.00 39.71 | | • | N |
| | MOTA | 12602 | N | GLY C | 34 | | 38.621 | 21.204 | 61.713 | 1.00 45.14 | | | C |
| 15 | MOTA | 12604 | CA | GLY C | 34 | | 38.955 | 20.018 | 62.634 | 1.00 44.20 | | | С |
| | ATOM | 12607 | C | GLY C | 34 | | 38.190 | 19.062 | 62.710 | 1.00 44.56 | | | 0 |
| | MOTA | 12608 | 0 | GLY C | 34 | | 40.102 | 20.086 | 63.318 | 1.00 39.94 | | | N |
| | ATOM | 12609 | N | SER C | 35. | | | 19.124 | 64.357 | 1.00 36.97 | | | C |
| | ATOM | 12611 | CA | SER C | 35 | | 40.490 | 17.909 | 63.768 | 1.00 41.17 | | | С |
| 20 | MOTA | 12613 | CB | SER C | 35 | | 41.195 | 18.109 | 63.530 | 1.00 39.49 | | | ο. |
| | MOTA | 12616 | OG | SER C | 35 | | 42.575 | - | 65.385 | 1.00 41.65 | | | C |
| | MOTA | 12618 | С | SER C | 35 | | 41.423 | 19.799 20.986 | 65.259 | 1.00 38.82 | | | o |
| | ATOM | 12619 | 0 | SER C | 35 | | 41.747 | | 66.384 | 1.00 41.66 | | | N |
| | ATOM | 12620 | N | SER C | 36 | | 41.881 | 19.044 | 67.476 | 1.00 36.97 | | | C |
| 25 | ATOM | 12622 | CA | SER C | 36 | • | 42.683 | 19.621 | | 1.00 30.37 | | | Ċ |
| | MOTA | 12624 | CB | SER C | 36 | | 41.755 | 19.879 | 68.673 | 1.00 33.43 | | | ō |
| - | MOTA | 12627 | OG | SER C | 36 · | | 40.776 | 20.894 | 68.393 67.975 | 1.00 34.74 | | | č |
| | MOTA | 12629 | C | SER C | 36 | | 43.908 | | | 1.00 46.46 | | | ŏ |
| | MOTA | 12630 | 0 | SER C | 36 | | 44.478 | 19.169 | 69.000 | 1.00 48.40 | | | N |
| 30 | MOTA | 12631 | N | ASN C | 37 | | 44.322 | 17.742 | 67.298 | 1.00 34.35 | | | c |
| | MOTA | 12633 | CA | ASN C | 37 | | 45.511 | 17.024 | 67.723 | 1.00 38.23 | | | Ç |
| | ATOM | 12635 | CB | ASN C | -37 | | 45.259 | 15.525 | 67.766 | 1.00 38.28 | | | č |
| | MOTA | 12638 | CG | ASN C | 37 | | 44.338 | 15.132 | 68.855 | | | | ŏ |
| • | ATOM | 12639 | | ASN C | 37 | | 43.120 | | 68.681 | 1.00 38.23 | | | N |
| 35 | MOTA | 12640 | ND2 | ASN C | 37 | | 44.911 | 14.815 | 69.992 | 1.00 37.80 | | | C |
| | MOTA | 12643 | С | ASN C | | | 46.674 | 17.175 | 66.771 | 1.00 37.54 1.00 34.71 | | | ŏ |
| | MOTA | 12644 | 0 | ASN C | | | 46.475 | 17.306 | 65.578 | | | | N |
| | MOTA | 12645 | N | PHE C | 38 | | 47.888 | 17.150 | 67.322 | 1.00 35.88 | | | c |
| | MOTA | 12647 | CA | PHE C | | | 49.090 | 17.051 | 66.525 | 1.00 33.22 1.00 31.39 | | | č |
| 40 | MOTA | 12649 | CB | PHE C | | | 50.203 | 17.902 | 67.126 | | | | ·C |
| | MOTA | 12652 | CG | PHE C | | | 51.541 | 17.943 | 66.303 | 1.00 37.60 1.00 37.64 | | | C |
| | MOTA | 12653 | CD: | L PHE C | | | 52.748 | | 66.931 | | | | č |
| | MOTA | 12655 | CE. | L PHE C | | | 53.864 | | 66.256 | 1.00 42.48 | | | Č |
| | ATOM | 12657 | CZ | PHE C | | | 53.869 | | 64.938 | 1.00 41.33 | | | Ċ |
| 45 | ATOM | 12659 | CE: | 2 PHE C | | | 52.742 | | 64.307 | 1.00 43.17 | | | č |
| | ATOM | .12661 | CD: | 2 PHE C | : 38 | | 51.573 | | 64.979 | 1.00 38.57 | | | Ċ |
| | MOTA | 12663 | C | PHE C | | | 49.361 | | | 1.00 31.89 | | | ő |
| • | ATOM | 12664 | 0 | PHE C | 38 | | 49.328 | | | | - | | N |
| | MOTA | 12665 | · N | ALA (| 39. | | 49.584 | | | | | | C |
| 50 | ATOM | | | ALA (| 39 | | 49.777 | 13.542 | | | | | C |
| | MOTA | | | ALA (| 39 | | 48.450 | | | | | | C |
| • | ATOM | | С | ALA (| 39 | | 50.557 | | | | | | o |
| | ATOM | | | ALA (| 39 | | 50.252 | | | | | | |
| | ATOM | | | VAL | 2 40 | | 51.556 | | | | , | | N |
| 55 | ATOM | | | • | | | 52.402 | | | | • | | C |
| | ATOM | | | | | | 53.865 | | | 1.00 51.51 | | | C |
| | ATOM | | | 1 VAL | | | 54.002 | | | | | | C |
| | ATOM | | | 2 VAL | | | 54.444 | | | | | | C |
| | ATOM | | | VAL | | | 52.504 | | | | | | C |
| 60 | | | | VAL | | | 52.333 | | | | • | | 0 |
| UU | ATOM | | | GLY | | | 52.79 | 6 10.017 | 61.429 | 1.00 42.10 | | | N |
| | W.O. | | | . — — | _ | | • | | | | | | |

| | | → , | | | | | | 004 | 8.600 | 61.217 | 1.00 | 36.51 | | | С |
|----|-------|------------|-----|------|-----|------|----|----------------|-------|----------|-------|---------|---|----|------------|
| 5 | ATOM | 12693 | | GLY | | 41 | | 024 | | 61.900 | 1 00 | 45.89 | | | С |
| | MOTA | 12696 | | GLY | | 41 | | .331 | 8.220 | | | 41.98 | • | | Ō |
| • | | 12697 | 0 | GLY | С | 41 | | 312 | 8.941 | 61.803 | | | • | | N |
| | ATOM | 12698 | N | ALA | С | 42 | | . 368 | 7.083 | 62.591 | 1.00 | 49.43 | | | C |
| | ATOM | 12700 | CA | ALA | С | 42 | | . 588 | 6,687 | 63.291 | | 46.63 | | | c |
| 10 | MOTA | 12702 | CB | ALA- | С | 42 | 55 | . 434 | 6.999 | 64.733 | | 44.75 | | | |
| 10 | | 12706 | C | ALA | | 42 | 55 | .868 | 5.196 | 63.096 | 1.00 | 50.91 | | | С |
| | ATOM | 12707 | Ö | ALA | | 42 | 56 | .415 | 4.512 | 63.968 | 1.00 | 56.15 | | | 0 |
| | ATOM | | N | ALA | | 43 | | . 494 | 4.714 | 61.923 | | 51.91 | | | N |
| | MOTA | 12708 | | ALA | | 43 | | .530 | 3.302 | 61.647 | | 55.01 | | | С |
| · | MOTA | 12710 | CA | | | 43 | | .578 | 2.588 | 62.522 | 1.00 | 56.93 | | ٠. | С |
| 15 | MOTA | 12712 | CB | ALA | | | | .118 | 3.057 | 60.232 | 1.00 | 59.43 | * | | C |
| | MOTA | 12716 | С | ALA | | 43 | | .070 | 3.538 | 59.772 | | 58.38 | | | 0 |
| | ATOM | 12717 | 0 | ALA | | 43 | | | 2.315 | 59.555 | 1.00 | 59.53 | | | N |
| | MOTA | 12718 | N · | PRO | | 44 | | .971 | | 58.207 | 1 00 | 57.91 | | | С |
| | ATOM | 12719 | ·CA | PRO | | 44 | | .738 | 1.800 | 58.373 | | 58.24 | | | C |
| 20 | MOTA | 12721 | CB | PRO | | 44 | | .185 | 0.392 | | | 60.25 | | | C . |
| | ATOM | 12724 | CG | PRO | С | 44 | | .450 | 0.628 | 59.193 | | 59.83 | | | C |
| | ATOM | 12727 | CD | PRO | С | 44 | | .296 | 1.930 | | | | • | | Ċ. |
| | ATOM | 12730 | C | PRO | C | 44 | | .345 | 1.869 | 57.679 | | 51.08 | | • | o |
| | ATOM | 12731 | o | PRO | С | 44 | 53 | .427 | 1.440 | 58.331 | | 42.11 | | | |
| 25 | ATOM | 12732 | N | HIS | | 45 | 54 | .228 | 2.439 | 56.483 | | 51.18 | | | N |
| 23 | ATOM | 12734 | CA | HIS | | 45 | 52 | .943 | 2.516 | 55.767 | | 51.14 | | | С |
| | | 12736 | СВ | HIS | | 45 | 51 | .987 | 3.544 | 56.361 | | 49.59 | | | С |
| | ATOM | | CG | HIS | | 45 | 50 | .664 | 3.623 | 55.641 | | 55.41 | | | C |
| | ATOM | 12739 | | HIS | | 45 | | .552 | 4.007 | 54.318 | | 50.15 | | | N |
| • | MOTA | 12740 | | HIS | | 45 | | .280 | 3.983 | 53.961 | 1.00 | 48.42 | | | C |
| 30 | ATOM | 12742 | | HIS | | 45 | | 3.563 | 3.582 | 54.993 | 1.00 | 48.32 | | | N |
| | MOTA | 12744 | | | | 45 | | 3.401 | 3.351 | 56.058 | | 50.46 | | | С |
| | ATOM | 12746 | | HIS | | | | 3.171 | 2.803 | 54.287 | | 51.98 | | | C |
| | ATOM | 12748 | С | HIS | | 45 | | | 3.610 | 53.912 | | 58.52 | | | 0 |
| | ATOM | 12749 | 0 | HIS | | 45 | | 3.986 2.430 | 2.123 | 53.444 | | 59.22 | | | N |
| 35 | MOTA | 12750 | N | PRC | | 46 | | | 2.244 | 51.977 | | 58.93 | | | C |
| | MOTA | 12751 | CA | PRC | | 46 | | 2.535 | 1.382 | | | 60.36 | | | С |
| | MOTA | 12753 | СB | PRO | | 46 | | 1.381 | | 52.553 | | 62.16 | | | С |
| | MOTA | 12756 | CG | PRO | | 46 | | 1.169 | 0.420 | 53.851 | | 58.40 | | | С |
| | MOTA | 12759 | CD | PRO | | 46 | , | 1.412 | 1.141 | | | 60.75 | | | Ċ |
| 40 | MOTA | 12762 | С | PRO | | 46 | | 2.263 | | 51.375 | | 66.57 | | | ō |
| - | ATOM | 12763 | 0 | PRO | C | 46 | | 2.429 | 3.742 | | | | | | N |
| | ATOM | 12764 | N | PHI | E C | 47 | | 1.820 | 4.582 | | | 53.51 | | | C |
| | MOTA | 12766 | CA | PHI | E C | 47 | 5 | 1.687 | 5.885 | | | 54.37 | | | Ċ |
| | ATOM | 12768 | CB | PHI | E C | 47 | 5 | 0.227 | 6.362 | | | 55.83 | | | c |
| 45 | ATOM | | CG | PH | E C | 47 | 4 | 9.248 | 5.477 | 50.798 | | 56.85 | | • | |
| | ATOM | | | 1 PH | E C | 47 | 4 | 7.889 | 5.498 | | | 53.21 | | | С |
| | ATOM | | CE | 1 PH | E C | 47 | 4 | 7.022 | 4.712 | 50.358 | | 0 58.68 | | | C |
| | ATOM | | | PH | | | 4 | 7.494 | 3.872 | | | 0 53.11 | | | C |
| | ATOM | | | 2 PH | E C | 47 | 4 | 8.802 | 3.834 | 49.068 | 1.0 | 0 53.10 | | • | C. |
| 50 | | | | 2 PH | | | | 9.693 | 4.630 | | | 0 59.43 | | | С |
| 50 | ATOM | | | | EC | | | 2.728 | | | 1.0 | 0 53.35 | | | C |
| | ATOM | | | | | | | 2.739 | 8.075 | | | 0 47.38 | | | 0 |
| | ATOM | | | | E C | | | 3.602 | | | | 0 47.46 | | | N |
| | ATOM | | | 7.5 | U C | 48 | | 4.627 | 7.217 | | | 0 48.00 | | | С |
| | ATOM | | | | U C | | | | 6.868 | | | 0 44.63 | | | . C |
| 55 | ATOM | | | | U C | | | 4.585 | | | | 0 36.89 | | | С |
| | ATOM | | | | ט כ | | | 3.203 | 7.093 | | | 0 32.35 | | • | Č |
| | ATOM | | | 1 LE | | | | 3.226 | 7.095 | | | | | | č |
| | .ATOM | | | 2 LE | | | | 2.716 | | | | 0 43.78 | | | Č |
| | ATOM | | | | U C | | | 6.055 | | | | 0 49.23 | | | ŏ |
| 60 | ATOM | | | | U C | | | 6.512 | | | | 0 51.31 | | | N |
| | ATOM | | | HJ | s c | 2 49 | | 56.741 | 8.082 | 2 52.772 | 4 1.0 | 0 54.74 | | | 14 |
| | | | | | | | | | | | | | | | |

| - | | | ~~ | | 49 | | 58.138 | 8.036 | 52.290 | 1.00 5 | 5.16 | | | C |
|------|---|-------|-----|-------|------------|---|--------|--------|--------|--------|----------------|---|---|-----|
| 5 | • | 12805 | | HIS C | | | 58.563 | 9.276 | 51.513 | 1.00 € | 2.74 | | | С |
| | ATOM | 12807 | | HIS C | 49 | | | 9.479 | 50.216 | 1.00 8 | 0.32 | | | C . |
| | MOTA | 12810 | | HIS C | 49 | | 57.851 | | | 1.00 | 0 23 | | | N |
| | MOTA | 12811 | | HÌS C | | | 57.953 | 8.596 | 49.157 | 1.00 | 0.25 | | | C |
| | MOTA | 12813 | CE1 | HIS C | 49 | | 57.221 | 9.041 | 48.148 | 1.00 | 0.05 | | | N |
| 10 | MOTA | 12815 | NE2 | HIS C | 49 | | 56.653 | 10.180 | 48.512 | 1.00 8 | | | | |
| 10 | ATOM | 12817 | | HIS C | | | 57.032 | 10.477 | 49.799 | 1.00 8 | 35.00 | | | С |
| | | 12819 | | HIS C | | | 58.985 | 8.110 | 53.491 | 1.00 5 | 52.56 | | | C |
| | MOTA | 12820 | | HIS C | | | 60.083 | 7.550 | 53.529 | 1.00 | 57.27 | | | 0 |
| | MOTA | | | ARG C | | | 58.495 | 8.859 | 54.472 | 1.00 | 16.86 | | | N |
| | MOTA | 12821 | | ARG C | | | 59.152 | 8.928 | 55.749 | 1.00 | 44.15 | | | С |
| 15 | MOTA | 12823 | | | | | 60.123 | 10.094 | 55.776 | 1.00 | 47.15 | | | С |
| | MOTA | 12825 | | ARG C | | | | 11.362 | 55.346 | 1.00 | | | | С |
| | MOTA | 12828 | | ARG C | | | 59.543 | 12.504 | 55.358 | 1.00 | | | | C |
| | MOTA | 12831 | CD | ARG C | | | 60.498 | | | 1.00 | 57 92 | | | N |
| | ATOM | 12834 | NE | ARG C | | | 59.733 | 13.667 | 54.935 | 1.00 | | | | C |
| 20 | ATOM | 12836 | CZ | ARG C | 50 | | 60.210 | 14.894 | 54.724 | 1.00 | 51.10 C1 00 | | | Ŋ |
| | ATOM | 12837 | NH1 | ARG C | 50 | | 61.491 | 15.192 | 54.882 | 1.00 | | | | |
| • | ATOM | 12840 | | ARG C | | | 59.366 | 15.835 | 54.342 | 1.00 | | | | N |
| | MOTA | 12843 | С | ARG C | | | 58.192 | 9.000 | 56.918 | 1.00 | | | | С |
| | | 12844 | ō | ARG C | | | 56.992 | 9.149 | 56.762 | 1.00 | | | | 0 |
| 05 | ATOM | | N | TYR C | | | 58.746 | 8.873 | 58.107 | 1.00 | 43.42 | | | N |
| 25 | ATOM | 12845 | | | | | 57.961 | 8.988 | 59.304 | 1.00 | 46.93 | | | С |
| • | MOTA | 12847 | CA | TYR C | | • | 57.068 | 7.774 | 59.414 | 1.00 | | | | C |
| | MOTA | 12849 | CB | TYR C | | | | 6.503 | 59.490 | | 57.25 | | | C |
| | MOTA | 12852 | CG | TYR C | | | 57.838 | | 60.706 | 1.00 | | | • | С |
| | MOTA | 12853 | | TYR C | | | 58.167 | 5.944 | | | 64.00 | | | C |
| 30 | MOTA | 12855 | CE1 | TYR C | | | 58.876 | 4.753 | 60.768 | 1.00 | 65.22 | | | Ċ |
| | MOTA | 12857 | CZ | TYR (| 51 | | 59.260 | 4.118 | 59.593 | | | | | ō |
| | ATOM | 12858 | OH | TYR (| 51 | | 59.966 | 2.928 | 59.626 | | 68.18 | • | | c |
| | ATOM | 12860 | CE2 | TYR (| 51 | | 58.939 | 4.662 | 58.380 | | 61.62 | | • | |
| | ATOM | 12862 | | TYR (| | | 58.236 | 5.844 | 58,331 | | 62.51 | | | С |
| 35 | ATOM | 12864 | C | TYR (| | | 58.822 | 9.143 | 60.563 | | 40.91 | | ٠ | С |
|)) | ATOM | 12865 | ō | TYR | | | 59.999 | 8.948 | 60.522 | | 42.94 | | | 0 |
| | | 12866 | N | TYR | | | 58.190 | 9.503 | 61.674 | 1.00 | 40.91 | | | N |
| | MOTA | | CA | TYR | | | 58.832 | 9.726 | 62.976 | 1.00 | 40.27 | | | С |
| | ATOM | 12868 | | TYR | | | 57.747 | 10.233 | 63.886 | 1.00 | 41.76 | | | С |
| 40 | ATOM | 12870 | CB | | | | 58.122 | 10.764 | 65.232 | | 41.11 | | | С |
| 40 | ATOM | 12873 | CG | TYR | | | 59.174 | 11.588 | 65.399 | | 47.30 | | | С |
| | MOTA | 12874 | | TYR | | | | 12.084 | 66.637 | | 50.41 | | | С |
| | MOTA | 12876 | | TYR | | | 59.492 | | 67.719 | | 49.29 | | | С |
| | ATOM | 12878 | CZ | TYR | | | 58.750 | 11.768 | | | 53.62 | | | ō |
| | MOTA | 12879 | OH | TYR | | | 59.121 | 12.304 | 68.943 | | 46.11 | | | c |
| 45 | MOTA | 12881 | CE2 | TYR | | | 57.685 | 10.943 | | | | | | č |
| | ATOM | 12883 | CD2 | TYR | C 52 | 2 | 57.377 | 10.449 | | | 46.35 | | | c |
| | ATOM | 12885 | - C | TYR. | C 52 | 2 | 59.394 | 8.525 | | • | 41.56 | | | |
| | ATOM | 12886 | | TYR | | 2 | 58.631 | 7.656 | 64.087 | | 42.35 | | | 0 |
| | ATOM | 12887 | N | GLN | | | 60.711 | 8.500 | 63.860 | 1.00 | 44.45 | | | N |
| 50 | | | | GLN | | | 61.404 | 7.421 | | 1.00 | 41.54 | | | C |
| . 50 | ATOM | | | GLN | | | 62.681 | | | | 44.38 | • | | C |
| | MOTA | | CB | | | | 62.440 | | | | 51.42 | • | | C |
| | MOTA | | CG | GLN | | | 63.227 | | | | 59.82 | | | C |
| | ATOM | | | GLN | | | | | | | 61.98 | | | 0 |
| | MOTA | | | LGLN | | | 63.842 | | | | 67.41 | | | N |
| . 55 | ATOM | 12899 | NE | 2 GLN | | | 63.204 | | | | | | | C |
| | ATOM | 12902 | С | GLN | | 3 | 61.698 | | | | 39.42 | | | 0 |
| | ATOM | | | GLN | C 5 | 3 | 62.595 | | | | 53.39 | | | |
| | ATOM | | | ARG | | | 60.926 | | | | 38.63 | • | | N |
| | ATOM | | | ARG | | | 61.004 | 7.780 | 68.276 | | 42.43 | | | C |
| 60 | ATOM | | | ARG | | 4 | 59.828 | | | 1.00 | 39.75 | | | С |
| UU | | | | ARG | | 4 | 58.574 | | | | 40.81 | | • | С |
| : | ATOM | 17271 | | טאת | U J | - | | 2 | • | | | | | |

| | | * | | | | | | | | | | | | | |
|-----|------|--------|-----|-------|------------|----------|---|---------|--------|--------|---------|-------|---|---|----|
| 5 | MOTA | 12914 | CD | ARG | С | 54 | | 57.389 | 7.431 | 69.538 | 1.00 39 | | | | С |
| • | ATOM | 12917 | NE | ARG | С | 54 | | 57.137 | 6.168 | 68.844 | 1.00 40 | | | | N |
| | ATOM | 12919 | CZ | ARG | | 54 | | 56.124 | 5.372 | 69.092 | 1.00 49 | 5.54 | | | С |
| | ATOM | 12920 | | ARG | | 54 | | 55.230 | 5.686 | 70.027 | 1.00 47 | 7.14 | | | N |
| | MOTA | 12923 | | ARG | | 54 | | 56.000 | 4.257 | 68.396 | 1.00 48 | | | | N |
| 10 | ATOM | 12926 | C | ARG | | 54 | | 62.219 | 7.302 | 69.005 | 1.00 4 | 7.24 | | | С |
| 10 | ATOM | 12927 | Ŏ | ARG | | 54 | | 62.621 | 7.870 | 70.013 | 1.00 49 | 9.66 | | | 0 |
| | ATOM | 12928 | N | GLN | | 55 | | 62.795 | 6.236 | 68.482 | 1.00 5 | 5.23 | | | N |
| | ATOM | 12930 | CA | GLN | | 55 | | 63.960 | 5.624 | 69.061 | 1.00 5 | 5.09 | | | С |
| | ATOM | 12932 | CB | GLN | | 55 | | 64.162 | 4.277 | 68.388 | 1.00 6 | 0.40 | | | С |
| 15 | ATOM | 12935 | CG | GLN | | 55 | | 64.836 | 4.423 | 67.025 | 1.00 6 | 2.46 | | | С |
| 15 | | 12938 | CD | GLN | | 55 | | 63.988 | 4.048 | 65.850 | 1.00 6 | | | | С |
| | MOTA | 12939 | | GLN | | 55 | | 64.541 | 3.682 | 64.814 | 1.00.6 | | | | 0 |
| | ATOM | | • | GLN | | 55 | | 62.663 | 4.155 | 65.977 | 1.00 5 | | | | N |
| • | ATOM | 12940 | | | | 55 | | 65.197 | 6.491 | 68.835 | 1.00 5 | | | | С |
| 20 | ATOM | 12943 | C. | GLN | | 55 55 | | 66.185 | | 69.567 | 1.00 5 | | | | 0 |
| 20 | ATOM | 12944 | 0 | GLN | | | | 65.157 | 7.368 | 67.828 | 1.00 5 | | | | N |
| • | ATOM | 12945 | N | LEU | | 56 | | 66.331 | 8.196 | 67.506 | 1.00 5 | | | | С |
| | ATOM | 12947 | CA | LEU | | 56 | | | 8.354 | 65.983 | 1.00 5 | | | | c |
| | MOTA | 12949 | СВ | LEU | | 56 | | 66.500 | 7.101 | 65.101 | 1.00 5 | | | | č |
| | MOTA | 12952 | CG | LEU | | 56 | | 66.445 | | | 1.00 4 | | | | č |
| .25 | MOTA | 12954 | | LEU | | 56 | | 66.780 | 7.437 | 63.654 | 1.00 4 | | | | č |
| | MOTA | 12958 | | LEU | | 56 | | 67.364 | 6.071 | 65.629 | | | | | c |
| | MOTA | 12962 | С | LEU | | 56 | | 66.333 | 9.594 | | 1.00 4 | | | | Ö |
| | MOTA | 12963 | 0 | LEU | | 56 | | 67.129 | 10.385 | 67.639 | 1.00 5 | | | | N |
| | MOTA | 12964 | N | SER | | 57 | | 65.453 | 9.904 | 69.012 | 1.00 4 | | | | C |
| .30 | MOTA | 12966 | CA | SER | | 57 | | 65.298 | 11.260 | 69.565 | 1.00 4 | | | | c |
| | MOTA | 12968 | CB | SER | | 57 | | 63.841 | 11.680 | 69.338 | 1.00 4 | | | | |
| | ATOM | 12971 | OG | SER | | 57 | | 63.487 | 12.916 | 69.932 | 1.00 4 | | | | 0 |
| | ATOM | 12973 | С | SER | | 57 | | 65.585 | 11.166 | 71.061 | 1.00 4 | | | | С |
| | MOTA | 12974 | 0 | SER | C | 57 | | 64.960 | 10.361 | 71.721 | 1.00 4 | | | | 0 |
| 35 | ATOM | 12975 | N | SER | C. | 58 | | 66.513 | 11.955 | 71.608 | 1.00 4 | | | | N |
| | MOTA | 12977 | CA | SER | | . 58 | | 66.828 | 11.885 | 73.068 | 1.00 4 | | | | С |
| | MOTA | 12979 | CB | SER | | 58 | | 68.186 | 12.471 | 73.363 | 1.00 3 | | | | С |
| | ATOM | 12982 | OG | SER | С | 58 | | 68.146 | 13.786 | 72.887 | 1.00 3 | | | | 0 |
| | MOTA | 12984 | ·C | SER | | 58 | | 65.869 | 12.689 | 73.911 | 1.00 4 | | | | C. |
| 40 | ATOM | 12985 | 0 | SER | С | 58 | | 65.676 | 12.433 | 75.101 | 1.00 4 | | • | | 0 |
| | ATOM | 12986 | N | THR | С | 59 | | 65.272 | 13.684 | 73.297 | 1.00 4 | | | | N |
| - | MOTA | 12988 | CA | THR | C | 59 | | 64.320 | 14.493 | 73.998 | 1.00 4 | | | | C |
| | ATOM | 12990 | CB | THR | C | 59 | | 64.257 | 15.835 | 73.328 | 1.00 3 | | | | C |
| | MOTA | 12992 | OG1 | THR | . C | 59 | | 63.953 | 15.610 | 71.960 | 1.00 4 | | | | 0 |
| 45 | ATOM | 12994 | CG2 | THR | . С | 59 | | 65.592 | 16.504 | 73.267 | 1.00 4 | | | | C |
| | ATOM | .12998 | С | THR | C | 59 | | 62.910 | 13.889 | 73.942 | 1.00 4 | | | | С |
| | ATOM | 12999 | 0 | THR | C | 59 | • | 61.953 | 14.574 | 74.329 | 1.00 | | | | 0 |
| | ATOM | 13000 | N | TYR | C | 60 | | 62.732 | 12.652 | 73.481 | 1.00 | | | | N |
| | ATOM | 13002 | CA | TYR | C | 60 | | 61.378 | 12.126 | 73.373 | 1.00 | | | | С |
| 50 | MOTA | 13004 | CB | | | 60 | | 61.255 | 11.078 | 72.235 | | | | | С |
| | ATOM | 13007 | CG | TYR | | 60 | | 60.194 | 10.045 | 72.509 | | | | | С |
| | ATOM | 13008 | | 1 TYR | | 60 | | 58.876 | 10.239 | 72.078 | 1.00 | 35.41 | | | С |
| | ATOM | 13010 | | L TYR | | 60 | | 57.873 | 9.308 | 72.344 | 1.00 | 37.20 | | | С |
| | ATOM | 13012 | CZ | TYP | | 60 | | 58.178 | 8.161 | 73.048 | 1.00 | 48.24 | | | С |
| 55 | ATOM | 13013 | OH | TYP | | 60 | | 57.188 | 7.246 | 73.312 | | | | | 0 |
| 23 | ATOM | 13015 | | 2 TYP | | 60 | | 59.496 | 7.934 | 73.495 | | | | • | С |
| | ATOM | | | 2 TYF | | 60 | | 60.496 | 8.895 | 73.223 | | | | | С |
| | ATOM | | | TYF | | 60 | | 61.040 | 11.487 | 74.690 | | | | | C |
| | ATOM | | | TYF | | | | 61.858 | 10.721 | 75.189 | | | | | 0 |
| 60 | MOTA | | | ARG | | | • | 59.843 | 11.823 | 75.211 | | | | | N |
| JU | | | | | | | | 59.216 | 11.303 | 76.438 | | | | | C |
| | ATOM | 13023 | CA | LILL | | OT | | JJ. 220 | | | | | | | |

| _ | | 15005 | an | 200 | _ | 6 i | 58.773 | 12.440 | 77.347 | 1.00 | 49.63 | | | С |
|------|------|---------|-----------|-------|------|------------|--------|--------|--------|------|---------|---|---|--------|
| 5 | ATOM | 13025 | CB | ARG | | | 59.774 | 12.823 | 78.369 | 1.00 | 60.48 | | | С |
| | MOTA | 13028 | CG | ARG | | 61 | 60.050 | 11.712 | 79.429 | | 66.22 | | | C |
| | MOTA | 13031 | CD | ARG | | 61 | 60.843 | 10.550 | 78.950 | | 69.25 | | | N |
| | MOTA | 13034 | NE | ARG | | 61 | 62.129 | 10.585 | 78.575 | | 73.53 | | | C |
| | ATOM | 13036 | CZ | ARG | | 61 | 62.123 | 11.717 | 78.591 | | 76.07 | • | | N |
| 10 | MOTA | 13037 | | ARG | | 61 | 62.719 | 9.472 | 78.174 | | 74.09 | | | N |
| | ATOM | 13040 | | ARG | | 61 | | 10.601 | 76.126 | | 46.33 | | | С |
| | MOTA | 13043 | С | ARG | | 61 | 57.932 | | 75.381 | | 41.21 | | • | 0 |
| • | ATOM | 13044 | 0 | ARG | | 61 | 57.148 | 9.431 | 76.724 | | 52.19 | | | N |
| | MOTA | 13045 | N | ASP | | 62 | 57.694 | 8.630 | 76.471 | | 53.39 | | | С |
| 15 | MOTA | 13047 | CA | ASP | | 62 | 56.483 | | 76.486 | | 54.99 | | | С |
| | MOTA | 13049 | CB | ASP | | 62 | 56.850 | 7.160 | 75.881 | | 58.08 | | | С |
| • | MOTA | 13052 | CG | ASP | | 62 | 55.795 | 6.279 | 75.822 | | 57.84 | | | 0 |
| | MOTA | 13053 | | ASP | | 62 | 54.599 | 6.664 | | | 62.01 | | | 0 |
| | MOTA | 13054 | OD2 | ASP | | 62 | 56.086 | 5.151 | 75.442 | | 52.07 | | | C |
| 20 | MOTA | 13055 | C | ASP | | 62 | 55.442 | 8.874 | 77.549 | | 48.18 | | | ō |
| | MOTA | 13056 | 0 | ASP | С | 62 | 55.779 | 8.845 | 78.699 | | 57.80 | | | N |
| | MOTA | 13057 | N | LEU | Ċ | 63 | 54.192 | 9.116 | 77.150 | | | | | Ċ |
| | MOTA | 13059 | CA | LEU | C | 63 | 53.075 | 9.402 | 78.057 | | 56.98 | | | c |
| | ATOM | 13061 | CB | LEU | С | 63 | 52.160 | 10.437 | 77.404 | | 57.29 | | | č |
| 25 | MOTA | 13064 | CG | LEU | С | 63 | 52.776 | 11.820 | 77.240 | | 58.93 | | | c |
| | ATOM | 13066 | CD1 | LEU | C | 63 | 51.756 | 12.771 | 76.610 | | 58.33 | | | C |
| | ATOM | 13070 | CD2 | LEU | С | 63 | 53.270 | 12.356 | 78.568 | | 56.05 | | | c |
| | ATOM | 13074 | C | LEU | С | 63 | 52.234 | 8.183 | 78.511 | 1.00 | 57.00 | | | Ö |
| | ATOM | 13075 | 0 | LEU | С | 63 | 51.489 | 8.276 | 79.475 | | 56.10 | | | N |
| 30 | ATOM | 13076 | N | ARG | C | 64 | 52.323 | 7.053 | 77.828 | | 60.31 | • | | C |
| | MOTA | 13078 | CA | ARG | C | 64 | 51.702 | 5.821 | 78.337 | | 63.72 | | | |
| | ATOM | 13080 | CB | ARG | C | 64 | 52.093 | 5.634 | 79.801 | | 66.02 | | | Ċ |
| | | 13083 | CG | ARG | C | 64 | 53.077 | 4.540 | 80.025 | | 71.85 | | | |
| • | ATOM | 13086 | CD | ARG | | 64 | 54.241 | 4.949 | 80.865 | | 76.21 | | | C |
| -35 | MOTA | 13089 | NE | ARG | | 64 | 55.478 | 4.473 | 80.255 | | 83.39 | | | N |
| | ATOM | 13091 | CZ | ARG | | 64 | 55.840 | 4.763 | 79.018 | | 86.32 | | | C |
| , | ATOM | 13092 | | l ARG | S C | 64 | 55.045 | 5.527 | 78.271 | | 87.82 | | | N |
| | ATOM | 13095 | | 2 ARC | | 64 | 56.989 | 4.300 | 78.528 | | 87.10 | | | N |
| | ATOM | 13098 | С | ARG | | 64 | 50.204 | | 78.293 | | 63.01 | | | С |
| 40 | ATOM | 13099 | . 0 | ARG | G C | 64 | 49.556 | | 79.292 | | 67.08 | | | O N |
| | ATOM | 13100 | · N | | s c | 65 | 49.639 | 6.056 | 77.135 | | 62.20 | | | |
| | ATOM | 13102 | CA | LY | s c | 65 | 48.203 | | 77.021 | | 56.21 | | | C |
| | ATOM | 13104 | CB | | s c | 65 | 47.742 | | 77.559 | | 53.38 | | | C |
| | ATOM | 13107 | ĊG | LY | s c | 65 | 46.223 | | | | 61.59 | | | C |
| 45 | ATOM | | | | s c | 65 | 45.772 | 8.749 | 78.771 | | 65.72 | | | C |
| . 13 | ATOM | | | | s c | 65 | 46.070 | 10.201 | 78.354 | | 68.02 | | | С |
| | ATOM | | | | s c | 65 | 45.991 | 11.186 | | | 69.89 | | | N |
| • | ATOM | | | | s c | 65 | 48.062 | 6.104 | | | 50.29 | | | C |
| | ATOM | | | | s c | 65 | 48.950 | 6.506 | 74.846 | | 0 42.57 | | | 0 |
| 50 | ATOM | | | | Y C | | 46.965 | 5.552 | 75.088 | | 0 53.19 | | | N |
| 50 | MOTA | | | | Y, C | | 46.748 | 5.388 | 73.668 | | 0 53.88 | | | C |
| | ATOM | | | | Y C | 2.2 | 45.712 | 6.406 | 73.280 | | 0 55.77 | | • | C |
| | ATOM | | | | Y C | | 44.967 | | 74.141 | 1.0 | 0 61.89 | | | 0 |
| | ATOM | | | | тc | | 45.654 | | 71.993 | | 0 52.57 | | | N |
| 55 | | | | | TC | | 44.753 | | | 1.0 | 0 52.31 | | | C |
| 55 | ATOM | | | | TC | | 45.48 | _ | | | 0 56.46 | | | С |
| | ATOM | | | 1 VA | | | 46.91 | | | | 0 61.44 | | | С |
| | ATOM | | | 52 VA | | | 44.79 | | | | 0 59.86 | | | С |
| | ATOM | | | | VP C | | 44.32 | | | | 0 45.56 | | | С |
| ۲۸ | ATOM | | | | YP C | | 45.00 | | | | 0 50.56 | | | 0 |
| 60 | MOTA | | | | r C | | 43.16 | | | | 0 46.81 | | | N |
| | ATOM | 1 13145 | 5 N | 1.1 | | , 00 | ,43.10 | | | | | | | |

| | | 1 | | | | | | | | | | | |
|-----|------|-------|-----|---------|------|---|--------|--------|--------|------------|---|---|-----|
| 5 | ATOM | 13147 | CA | TYR C | 68 | | 42.612 | 7.210 | 68.435 | 1.00 49.00 | | | С |
| _ | ATOM | 13149 | CB | TYR C | 68 | | 41.772 | 5.909 | 68.608 | 1.00 53.23 | | | С |
| | ATOM | 13152 | CG | TYR C | 68 | | 40.433 | 6.120 | 69.280 | 1.00 57.32 | | | С |
| | ATOM | 13153 | | TYR C | 68 | | 39.298 | 6.444 | 68.537 | 1.00 61.05 | | | С |
| | | 13155 | CE1 | TYR C | 68 | | 38.076 | 6.653 | 69.151 | 1.00 62.40 | | | С |
| •• | ATOM | | | TYR C | 68 | | 37.980 | 6.524 | 70.533 | 1.00 65.60 | | | С |
| 10 | ATOM | 13157 | CZ | | 68 | | 36.814 | 6.708 | 71.234 | 1.00 73.33 | | | 0 |
| | ATOM | 13158 | OH | TYR C | | | 39.076 | 6.200 | 71.277 | 1.00 68.48 | | | c · |
| | ATOM | 13160 | | TYR C | 68 | | | 6.000 | 70.658 | 1.00 61.58 | | | С |
| ٠. | ATOM | 13162 | CD2 | TYR C | 68 | • | 40.302 | | 68.011 | 1.00 45.30 | | | Ċ |
| | MOTA | 13164 | С | TYR C | 68 | | 41.731 | 8.358 | | 1.00 41.65 | | | ō |
| 15 | MOTA | 13165 | 0 | TYR C | | | 41.033 | 8.953 | 68.837 | 1.00 45.31 | | | Ŋ. |
| | MOTA | 13166 | N | VAL C | | | 41.749 | 8.698 | 66.735 | 1.00 40.69 | | | Ç |
| | MOTA | 13168 | CA | VAL C | 69 | | 40.903 | 9.802 | 66.283 | | | | C |
| | MOTA | 13170 | CB | VAL C | | | 41.736 | 11.055 | 66.122 | 1.00 38.52 | ٠ | | · c |
| | ATOM | 13172 | CG1 | VAL C | 69 | | 40.861 | 12.229 | 65.749 | 1.00 42.88 | | | |
| 20 | ATOM | 13176 | CG2 | VAL C | 69 | • | 42.426 | 11.348 | 67.410 | 1.00 38.40 | | | C |
| | MOTA | 13180 | С | VAL C | 69 | | 40.159 | 9.561 | 64.990 | 1.00 38.40 | • | | С |
| | MOTA | 13181 | 0 | VAL C | | | 40.759 | 9.309 | 63.978 | 1.00 36.05 | | | 0 |
| | ATOM | 13182 | N | PRO C | | | 38.837 | 9.625 | 65.047 | 1.00 41.06 | - | | ·N |
| | ATOM | 13183 | CA | PRO C | | | 37.978 | 9.597 | 63.862 | 1.00 41.06 | | | С |
| 25 | ATOM | 13185 | CB | PRO C | | | 36.731 | 8.856 | 64.378 | 1.00 39.33 | | | ·C |
| 23 | MOTA | 13188 | CG | PRO C | | | 36.868 | 8.792 | 65.844 | 1.00 34.86 | | | С |
| | ATOM | 13191 | CD | PRO C | | | 38.030 | 9.668 | 66.268 | 1.00 41.35 | | | С |
| | | 13191 | C | PRO C | | | 37.582 | 11.001 | 63.320 | 1.00 43.22 | | | С |
| | MOTA | 13194 | 0 | PRO C | | | 37.305 | 11.927 | 64.102 | 1.00 41.52 | • | | 0 |
| 20 | ATOM | | | | | | 37.561 | 11.119 | 61.985 | 1.00 48.43 | | | N |
| .30 | ATOM | 13196 | N | TYR C | | | 37.249 | 12.328 | 61.206 | 1.00 45.43 | | | С |
| ٠. | MOTA | 13198 | CA | | | | 38.446 | 12.615 | 60.317 | 1.00 47.57 | | | С |
| | ATOM | 13200 | CB | TYR C | | | 39.761 | 12.912 | 61.024 | 1.00 45.81 | | | С |
| | ATOM | 13203 | CG | TYR C | | | 39.761 | 14.125 | 61.636 | 1.00 46.17 | | | C |
| | ATOM | 13204 | | TYR C | | | | 14.358 | 62.268 | 1.00 46.12 | | | Č |
| 35 | ATOM | 13206 | | TYR | | | 41.203 | 13.407 | 62.281 | 1.00 42.63 | | | Č |
| | MOTA | 13208 | CZ | TYR C | | | 42.180 | | 62.893 | 1.00 42.50 | | | ŏ |
| | MOTA | 13209 | OH | TYR C | | | 43.393 | 13.608 | 61.683 | 1.00 42.30 | | | Č. |
| | MOTA | 13211 | | TYR | | | 41.963 | 12.246 | | 1.00 47.18 | | | c |
| | MOTA | 13213 | | TYR C | | | 40.770 | 11.993 | 61.062 | 1.00 47.10 | | | č |
| 40 | ATOM | 13215 | С | TYR C | | | 36.034 | | 60.270 | | | | Ö |
| • | MOTA | 13216 | 0 | TYR C | | | 35.606 | 10.915 | 60.053 | 1.00 45.82 | | | N |
| • | ATOM | 13217 | N | THR C | | | 35.456 | 13.081 | 59.683 | 1.00 47.92 | | • | C. |
| | ATOM | 13219 | CA | THR (| | | 34.356 | 12.805 | 58.760 | 1.00 45.15 | | | C |
| | MOTA | 13221 | CB | THR (| | | 34.027 | 14.021 | 57.966 | 1.00 40.98 | | | |
| 45 | MOTA | 13223 | | L THR (| | | 33.809 | 15.111 | 58.867 | 1.00 39.12 | | | . 0 |
| | ATOM | 13225 | CG2 | 2 THR C | C 72 | | 32.706 | 13.846 | 57.309 | 1.00 48.15 | | | C |
| | MOTA | 13229 | C | THR | | | 34.709 | 11.612 | 57.857 | 1.00 45.22 | | - | C |
| | MOTA | 13230 | 0 | THR (| C 72 | | 33.884 | 10.719 | 57.657 | 1.00 47.99 | | | 0 |
| | ATOM | 13231 | N | GLN (| € 73 | | 35.919 | 11.612 | 57.302 | 1.00 47.77 | | | N |
| 50 | ATOM | 13233 | CA | GLN (| C 73 | | 36.473 | 10.435 | 56.643 | 1.00 48.67 | | | Ċ |
| | ATOM | 13235 | CB | GLN (| | | 36.522 | 10.536 | 55.123 | 1.00 48.78 | | | C |
| • | ATOM | 13238 | CG | GLN | | | 35.190 | 10.873 | 54.510 | 1.00 58.10 | | | С |
| ~~ | ATOM | 13241 | CD | GLN (| | | 34.661 | 9.825 | 53.533 | 1.00 65.47 | | | С |
| | ATOM | 13242 | | 1 GLN | | | 34.197 | 10.163 | 52.435 | 1.00 72.75 | | | 0 |
| 55 | ATOM | 13243 | | 2 GLN | | | 34.701 | 8.555 | 53.939 | 1.00 71.25 | 1 | | N |
| | MOTA | | C | GLN | | | 37.866 | 10.291 | 57.206 | | | | C |
| | ATOM | _ | ŏ | GLN | | | 38.559 | 11.293 | 57.431 | | | | 0 |
| | ATOM | | N | GLY | | | 38.274 | 9.049 | | | | | N |
| | | | CA | | | | 39.616 | 8.758 | 57.943 | | | | С |
| 60 | MOTA | | | GLY. | | , | 39.679 | 8.620 | | | | | С |
| UU | MOTA | | 0 | | | , | 38.937 | 9.283 | | | | | 0 |
| | MOTA | 13254 | J | GLY | . /4 | | | | | | | | |
| | | | | | | | | | | | | | |

| | | | | | | | | • | | | |
|----|------|-------|-----|-------|-----|--------|--------|--------|------------|---|-----|
| 5 | MOTA | 13255 | N | LYS C | 75 | 40.548 | 7.729 | 59.907 | 1.00 42.25 | | N |
| ٠. | ATOM | 13257 | CA | LYS C | 75 | 40.894 | 7.639 | 61.306 | 1.00 40.58 | | C |
| | ATOM | 13259 | CB | LYS C | 75 | 39.809 | 6.919 | 62.124 | 1.00 48.07 | | С |
| | ATOM | 13262 | CG | LYS C | 75 | 39.614 | 5.420 | 61.883 | 1.00 48.51 | | С |
| | ATOM | 13265 | CD | LYS C | 75 | 38.232 | 4.997 | 62.417 | 1.00 56.60 | | С |
| 10 | MOTA | 13268 | CE | LYS C | 75 | 37.077 | 5.271 | 61.414 | 1.00 56.69 | | C |
| | ATOM | 13271 | NZ | LYS C | 75 | 36.653 | 4.074 | 60.594 | 1.00 52.24 | | N |
| | ATOM | 13275 | С | LYS C | 75 | 42.270 | 6.970 | 61.410 | 1.00 41.75 | | С |
| | ATOM | 13276 | 0 | LYS C | 75 | 42.739 | 6.338 | 60.471 | 1.00 36.13 | | O . |
| | ATOM | 13277 | N | TRP C | 76 | 42.928 | 7.114 | 62.547 | 1.00 40.64 | | Ŋ |
| 15 | ATOM | 13279 | CA | TRP C | 76 | 44.226 | 6.491 | 62.759 | 1.00 41.83 | | С |
| | ATOM | 13281 | СВ | TRP C | 76 | 45.383 | 7.434 | 62.347 | 1.00 46.53 | | С |
| | ATOM | 13284 | CG | TRP C | .76 | 45.243 | 8.876 | 62.701 | 1.00 48.68 | | С |
| | ATOM | 13285 | CD1 | TRP C | 76 | 44.953 | 9.877 | 61.845 | 1.00 52.07 | | C |
| | ATOM | 13287 | NE1 | TRP C | 76 | 44.909 | 11.087 | 62.505 | 1.00 48.68 | | N |
| 20 | ATOM | 13289 | CE2 | TRP C | 76 | 45.183 | 10.869 | 63.828 | 1.00 35.18 | | С |
| | ATOM | 13290 | CD2 | TRP C | 76 | 45.401 | 9.492 | 63.992 | 1.00 46.84 | | С |
| | ATOM | 13291 | | TRP C | 76 | 45.705 | 9.007 | 65.273 | 1.00 46.09 | | С |
| | ATOM | 13293 | | TRP C | 76 | 45.773 | 9.884 | 66.311 | 1.00 41.49 | | С |
| | ATOM | 13295 | CH2 | TRP C | 76 | 45.548 | 11.258 | 66.099 | 1.00 43.75 | | С |
| 25 | ATOM | 13297 | | TRP C | 76 | 45.254 | 11.751 | 64.859 | 1.00 38.46 | | C. |
| 20 | MOTA | 13299 | С | TRP C | 76 | 44.298 | 6.196 | 64.227 | 1.00 41.30 | | C. |
| | ATOM | 13300 | O. | TRP C | 76 | 43.547 | 6.756 | 65.015 | 1.00 44.46 | | 0 |
| • | ATOM | 13301 | Ŋ | GLU C | 77 | 45.182 | 5.313 | 64.634 | 1.00 45.94 | | N |
| | ATOM | 13303 | CA | GLU C | 77 | 45.296 | 5.053 | 66.052 | | | С |
| 30 | ATOM | 13305 | CB | GLU C | 7.7 | 44.775 | 3.663 | 66.408 | | • | С |
| 20 | ATOM | 13308 | CG | GLU C | 77 | 44.214 | 3.526 | 67.827 | 1.00 59.61 | ٠ | C, |
| | ATOM | 13311 | CD | GLU C | 77 | 43.153 | 2.429 | 67.948 | 1.00 63.65 | | С |
| | ATOM | 13312 | OE1 | GLU C | 77 | 42.966 | 1.729 | 66.889 | 1.00 61.90 | • | Ο. |
| | ATOM | 13313 | | GLU C | 77 | 42.540 | 2.277 | 69.099 | 1.00 61.88 | | 0 |
| 35 | ATOM | 13314 | С | GLU C | 77 | 46.744 | 5.240 | 66.353 | 1.00 44.15 | | C |
| | ATOM | 13315 | 0 | GLU C | 77 | 47.580 | 5.038 | 65.481 | 1.00 50.71 | | 0 |
| | MOTA | 13316 | N | GLY C | 78 | 47.044 | 5.661 | 67.572 | 1.00 45.58 | | N |
| | ATOM | 13318 | CA | GLY C | 78 | 48.423 | 5.866 | 67.994 | 1.00 45.17 | | С |
| | ATOM | 13321 | С | GLY C | 78 | 48.639 | 5.842 | 69.506 | 1.00 47.59 | | С |
| 40 | MOTA | 13322 | Ο | GLY C | 78 | 47.757 | 5.539 | 70.298 | 1.00 51.18 | | 0 |
| | ATOM | 13323 | .N | GLU C | 79 | 49.850 | 6.195 | 69.897 | 1.00 49.48 | | N |
| | ATOM | 13325 | CA | GLU C | 79 | 50.272 | 6.234 | | 1.00 48.73 | | C |
| | MOTA | 13327 | CB | GLU C | 79 | 51.404 | 5.178 | 71.418 | 1.00 56.64 | | C |
| | ATOM | 13330 | CG | GLU C | 79 | 51.511 | 4.299 | 70.145 | 1.00 57.50 | | C. |
| 45 | MOTA | 13333 | CD | GLU C | 79 | 52.118 | 2.920 | 70.337 | 1.00 61.57 | | C |
| | ATOM | 13334 | | GLU C | 79 | 51.371 | 1.881 | 70.186 | 1.00 64.71 | | 0 |
| | ATOM | 13335 | OE2 | GLU C | 79 | | 2.881 | 70.607 | 1.00 68.25 | | Ö |
| | MOTA | 13336 | C · | GLU C | 79 | 50.759 | | 71.503 | 1.00 47.19 | | C |
| | MOTA | | О | GLU C | 79 | 51.353 | 8.279 | 70.596 | 1.00 48.26 | | O. |
| 50 | ATOM | 13338 | N | LEU C | 80 | 50.507 | 8.280 | 72.669 | 1.00 42.10 | | N. |
| | ATOM | 13340 | CA | TEA C | .80 | 50.942 | 9.647 | 72.904 | 1.00 39.01 | | C |
| | ATOM | 13342 | CB | LEU C | 80 | 50.042 | 10.306 | 73.887 | 1.00 41.35 | | C |
| | MOTA | 13345 | CG | LEU C | | 48.580 | 10.390 | 73.740 | 1.00 42.44 | | · C |
| | MOTA | 13347 | CD1 | LEU C | 80 | 48.100 | 10.134 | 75.134 | 1.00 42.44 | | C |
| 55 | MOTA | 13351 | CD2 | FER C | | 48.212 | 11.816 | 73.219 | 1.00 38.22 | | С |
| | ATOM | 13355 | C | LEU C | 80 | 52.283 | 9.789 | | | • | C |
| | ATOM | 13356 | 0 | LEU C | 80 | 52.812 | | 74.152 | 1.00 41.89 | | 0 |
| | ATOM | | N | GLY C | | 52.791 | | 73.540 | | | N |
| | ATOM | | CA | GLY C | | 54.096 | | | | | C |
| 60 | ATOM | | | GLY C | | 54.408 | | | | - | C |
| | MOTA | | | GLY C | 81 | 53.588 | 13.564 | 73.363 | 1.00 41.07 | | O |
| | | | | | | | | | | | |

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55.593
                                             13.298
                                                     74.206
                                                             1.00 42.53
         13364
                      THR C 82
5
    MOTA
                 N
                                                             1.00 45.55
                                             14.658
                                     55.918
                                                     73.863
    MOTA
          13366
                 CA
                      THR C
                             82
                                             15.597
                                                             1.00 47.68
                                     55.774
                                                     75.028
                      THR C
                             82
    MOTA
          13368
                 CB
                                             15.384
                                     56.874
                                                     75.898
                                                             1.00 52.01
          13370
                  OG1 THR C
                             82
    MOTA
                                                             1.00 49.71
                            82
                                     54.529
                                             15.315
                                                     75.871
    MOTA
          13372
                 CG2 THR C
                                     57.341
                                                     73.407
                                                             1.00 46.27
                      THR C
                                             14.742
10
    ATOM
          13376
                 С
                            82
                                                             1.00 44.96
                                     58.187
                                             13.956
                                                     73.830
                             82
                      THR C
    MOTA
          13377
                  0
                                                             1.00 43.18
                                                                                  N
                                     57.616 15.725
                                                     72.551
                      ASP C
                            83
          13378
    MOTA
                 N
                                                            1.00 39.07
                                                                                  С
                     ASP C
                                     58.959
                                            15.904
                                                     72.074
          13380
                 CA
                             83
    MOTA
                                                     70.959 1.00 35.57
                                                                                  C
                                     59.194
                                             14.931
                     ASP C 83
    ATOM 13382
                  CB
                                             14.729
                                                     70.684
                                                             1.00 45.60
                                                                                  C
                                     60.621
          13385
                     ASP C 83
15
    MOTA
                  CG
                  OD1 ASP C 83
                                     61.426 15.599
                                                     71.102
                                                             1.00 43.07
                                                                                  0
          13386
    MOTA
                                                                                  0
                                     61.036
                                             13.724
                                                     70.063
                                                             1.00 50.85
    MOTA
          13387
                  OD2 ASP C 83
                                                     71.621
                                                             1.00 41.05
                                                                                  C
                                     59.095
                                             17.351
                      ASP C. 83
    MOTA
          13388
                  С
                                             18.100
                                                     71.679
                                                             1.00 44.03
                                                                                  0
                      ASP C
                            83
                                     58.131
    MOTA
          13389
                  0
20
          13390
                      LEU C
                             84
                                     60.277 17.758
                                                     71.173
                                                             1.00 41.47
                                                                                  N
    MOTA
                  N
                                                                                  С
                                                     70.752
                                                             1.00 40.67
                      LEU C
                                     60.484
                                             19.150
    MOTA
          13392
                  CA
                             84
                                    61.977 19.519
                                                             1.00 39.63
                                                                                  С
                                                     70.806
                      LEU C
                             84
     MOTA
          13394
                  CB
                                                             1.00 38.29
                                     62.501
                                             19.477
                                                     72.235
                                                                                  C
         -13397
                  CG
                      LEU C
                             84
     MOTA
                                     63.972
                                             19.866
                                                     72.384
                                                             1.00 41.18
           13399
                  CD1 LEU C
                             84
     MOTA
                                                     72.966
                                                             1.00 35.07
                                     61.664
                                             20.398
25
     MOTA
           13403
                  CD2 LEU C
                            84
                                             19.298
                                                     69.361
                                                             1.00 38.41
                                                                                  ·C
                                     59.986
                            84
          13407
                      LEU C
     MOTA
                  С
                      LEU C 84
                                    60.002
                                             18.363
                                                    .68,623
                                                             1.00 46.50
                                                                                  0
          13408
                  0
    ATOM
                                                     68.990
                                                             1.00 42.93
                                                                                  N
                                     59.563
                                             20.484
          13409
                      VAL C 85
     MOTA
                  N
                                             20.699
                                                     67.676
                                                            1.00 43.40
                                                                                  C
                      VAL C 85
                                     59.011
          13411
    MOTA
                  CA
                                                             1.00 46.20
                                     57.500
                                             20.553
                                                     67.711
                                                                                  C
                      VAL C 85
30
    ATOM
          13413
                  CB
                                                     66.352
                                                             1.00 46.59
                                             20.747
                                                                                  С
           13415
                  CG1 VAL C 85
                                     56.968
     MOTA
                                                             1.00 45.29
                                     57.087
                                             19.179
                                                     68.253
                  CG2 VAL C 85
     MOTA
          13419
                                             22.100
                                                     67.248
                                                             1.00 45.84
                      VAL C 85
                                     59.260
     MOTA
          13423
                  С
                                                             1.00 51.25
                      VAL C 85
          13424
                                     58.967
                                             23.024
                                                     68.017
                                                                                   O
     MOTA
                  0
                                  59.787
                                             22.268
                                                     66.035
                                                             1.00 46.65
35
                      SER C
                            86
    MOTA
          13425
                  N
                                             23.583
                                                             1.00 43.45
                                     60.049
                                                     65.454
                                                                                   C
     ATOM
           13427
                      SER C 86
                  CA
                      SER C 86
                                     61.523
                                             23.738
                                                     65.141
                                                             1.00 49.82
                                                                                   C
     MOTA
          13429
                  CB
                      SER C 86
                                                     65.709
                                                             1.00 55.85
                                     62.315
                                             22.686
     MOTA
          13432
                  OG.
                      SER C 86
                                     59.319
                                             23.747
                                                     64.148
                                                             1.00 46.29
          13434
                  С
     ATOM
40
                      SER C 86
                                     58.902
                                             22.798
                                                     63.540
                                                            1.00 51.68
                                                                                   O
     MOTA
          13435
                  0
                                                     63.700
                                                                                   N
                                     59.125 24.972
                                                            1.00 52.23
     ATOM
          13436
                      ILE C 87
                                                     62.345
                                                                                   C
                      ILE C 87
                                     58.619 25.168
                                                            1.00 49.09
     ATOM
          13438
                  CA
                                     57.218
                                             25.802
                                                     62.337
                                                             1.00 45.63
                  CB
                      ILE C 87
     ATOM
          13440
                                                     63.533
                                                             1.00 45.33
                  CG1 ILE C 87
                                     56.382
                                             25.334
     ATOM
           13442
45
                            87
                                     54.875 25.472
                                                     63.339
                                                             1.00 45.27
     MOTA
           13445
                  CD1 ILE C
                                     56.523 25.509
                                                     61.022
                                                             1.00 47.91
                                                                                 · C
                  CG2 ILE C
                            87
     ATOM
           13449
                                     59.645
                                                     61.570 1.00 49.56
                                                                                   C
     MOTA
           13453
                      ILE C
                            87
                                             25.999
                  С
                                                     61.765 1.00 58.01
                                     59.723
                                             27.206
                            87
     MOTA
           13454
                  0
                      ILE C
                            88
                                     60.434
                                             25.374
                                                     60.701
                                                             1.00 50.26
           13455
     MOTA
                  N
                      PRO C
                      PRO C 88
                                     61.496
                                             26.064 59.944
                                                             1.00 51.41
50
           13456
     MOTA
                  CA
                                             25.005
                                                             1.00 51.62
                                                                                   С
                                     61.956
                                                     58.920
           13458
                      PRO C 88
     MOTA
                  CB
                                   61.429
                                                                                   С
          13461
                                             23.694
                                                     59.411
                                                             1.00 48.25
                      PRO C 88
     MOTA
                  CG
                                                                                   С
                      PRO C 88.
                                     60.353
                                             23.944
                                                     60.378
                                                             1.00 48.79
     ATOM
          13464
                  CD
                                                                                   C
           13467
                      PRO C 88
                                     61.054
                                             27.350
                                                     59.206
                                                             1.00 52.93
     MOTA
                  С
55
                                     61.716
                                             28.356
                                                     59.329
                                                             1.00 52.58
                                                                                   0
     MOTA
           13468
                  0
                      PRO C 88
                                             27.330
                                    59.970
                                                     58.447
                                                             1.00 52.36
                                                                                   N
           13469
                      HIS C 89
     MOTA
                  N
                      HIS C 89
                                     59.525
                                             28.548
                                                     57.787
                                                             1.00 50.37
           13471
     MOTA
                  CA
                                     59.057
                                             28.232
                                                     56.379
     ATOM
           13473
                  CB
                      HIS C
                             89
                                                              1.00 50.86
                                     60.154
                                             27.730
                                                     55.490
                                                              1.00 56.99
     MOTA
           13476
                  CG
                      HIS C
                             89
                                     61.204
                                                      55.084
           13477
                  ND1 HIS C
                             89
                                             28.524
                                                             1.00 62.43
     MOTA
                                     62.012
                                             27.830
     ATOM
           13479
                  CE1 HIS C 89
                                                     54.307
                                                             1.00 57.84
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| 5 | ATOM | 13481 | | HIS C | | | 61.528 | 26.610 | 54.196 | 1.00 56.97 | | | N |
|----|--------------|-------|------|-------|------|---|--------|--------|--------|------------|-----|---|----|
| | MOTA | 13483 | CD2 | HIS C | 89 | | 60.368 | 26.521 | 54.928 | 1.00 59.06 | | | C |
| | MOTA | 13485 | С | HIS C | 89 | | 58.422 | 29.176 | 58.631 | 1.00 50.27 | | | С |
| | ATOM | 13486 | 0 | HIS C | 89 | | 57.299 | 29.343 | 58.186 | 1.00 51.95 | | | 0 |
| | ATOM | 13487 | N | GLY C | | | 58.780 | 29.525 | 59.865 | 1.00 51.98 | | • | N |
| 10 | | 13489 | CA | GLY C | | | 57.866 | 30.031 | 60.882 | 1.00 49.95 | | | С |
| 10 | ATOM | 13492 | C | GLY C | | | 58.685 | 30.687 | 61.980 | 1.00 47.79 | | | С |
| | ATOM | | | GLY C | | | 59.913 | 30.701 | 61.889 | 1.00 57.85 | | | 0 |
| | MOTA | 13493 | 0 | | | | 58.029 | 31.167 | 63.034 | 1.00 42.33 | | | N |
| | ATOM | 13494 | N | PRO C | | | | | 63.990 | 1.00 45.30 | | | Ċ. |
| | MOTA | 13495 | CA | PRO C | | | 58.688 | 32.056 | 64.952 | 1.00 43.17 | • | | Č |
| 15 | MOTA | 13497 | CB | PRO C | | | 57.586 | 32.447 | | 1.00 41.44 | | | c |
| | MOTA | 13500 | CG | PRO C | | | 56.415 | 31.674 | 64.623 | 1.00 45.00 | • • | | c |
| | MOTA | 13503 | CD | PRO C | | | 56.658 | 30.820 | 63.433 | | | | C |
| | MOTA | 13506 | С | PRO C | | | 59.751 | 31.213 | 64.620 | 1.00 48.09 | | | |
| | MOTA | 13507 | 0 | PRO C | 91 | | 59.535 | 30.024 | 64.624 | 1.00 54.44 | | | 0 |
| 20 | MOTA | 13508 | N | GLN C | 92 | | 60.843 | 31.737 | 65.131 | 1.00 53.59 | | | N |
| | ATOM | 13510 | CA - | GLN C | 92 | | 61.921 | 30.814 | 65.443 | 1.00 59.67 | | | С |
| | ATOM | 13512 | CB | GLN C | 92 | | 63.309 | 31.354 | 65.139 | 1.00 62.99 | · | | С |
| | ATOM | 13515 | CG | GLN C | | | 63.355 | 32.565 | 64.259 | 1.00 69.98 | | | С |
| | ATOM | 13518 | CD | GLN C | | | 64.686 | 32.618 | 63.546 | 1.00 76.93 | | • | С |
| 25 | ATOM | 13519 | | | | | 65.246 | 31.554 | 63.191 | 1.00 79.49 | | | 0 |
| 23 | ATOM | 13520 | | GLN C | | | 65.210 | 33.837 | 63.335 | 1.00 74.23 | | | N. |
| | | 13523 | C | GLN C | | , | 61.893 | 30.449 | 66.851 | 1.00 59.04 | | | С |
| | ATOM | | | GLN C | | | 62.643 | 30.978 | 67.638 | 1.00 67.08 | | | 0 |
| | ATOM | 13524 | 0 | VAL | | | 61.035 | 29.507 | 67.152 | 1.00 57.44 | | | N |
| 20 | ATOM | 13525 | N | | | | 60.894 | 29.057 | 68.483 | 1.00 58.21 | | | C |
| 30 | ATOM | 13527 | CA | VAL C | | | 59.535 | 29.387 | 68.986 | 1.00 60.39 | | | Ċ |
| | MOTA | 13529 | СВ | VAL C | | | | | | 1.00 64.36 | | | C. |
| | ATOM | 13531 | | VAL C | | | 59.427 | 30.878 | 69.168 | 1.00 60.84 | | | Ċ. |
| | MOTA | 13535 | | VAL C | | | 58.494 | 28.878 | 68.008 | | | | Ċ. |
| | ATOM | 13539 | С | VAL | | | 61.032 | 27.581 | 68.473 | 1.00 59.93 | | | Ö. |
| 35 | ATOM | 13540 | 0 | VAL (| | | 61.183 | 26.945 | 67.436 | 1.00 63.78 | • | | |
| • | MOTA | 13541 | N | THR | | | 60.970 | 27.039 | 69.664 | 1.00 60.01 | | | N |
| | MOTA | 13543 | CA | THR (| | | 61.045 | 25.637 | 69.862 | 1.00 58.54 | | • | C. |
| | · ATOM | 13545 | CB | THR (| | | 62.448 | 25.299 | 70.252 | 1.00 59.14 | | | C |
| | ATOM | 13547 | OG1 | THR (| C 94 | | 63.337 | 26.190 | 69.577 | 1.00 65.27 | | | 0 |
| 40 | MOTA | 13549 | CG2 | THR (| C 94 | | 62.847 | 23.941 | 69.736 | 1.00 60.54 | | | C |
| | MOTA | 13553 | С | THR (| C 94 | | 60.123 | 25.447 | 71.023 | 1.00 59.67 | | | C. |
| | ATOM | 13554 | . 0 | THR (| C 94 | | 60.260 | 26.139 | 72.029 | 1.00 64.36 | | | 0 |
| | ATOM | 13555 | N | VAL (| C 95 | | 59.170 | 24.539 | 70.905 | 1.00 55.96 | | | N |
| | ATOM | 13557 | CA | VAL | C 95 | | 58.299 | 24.281 | 72.036 | 1.00 52.71 | • | | C |
| 45 | ATOM | 13559 | CB | VAL | C 95 | | 56.881 | 24.835 | 71.815 | 1.00 49.07 | | | С |
| | ATOM | | | VAL | C 95 | | 56.947 | 26.091 | 71.056 | 1.00 53.95 | • | | С |
| | ATOM | 13565 | | VAL (| | | 56.065 | 23.897 | 71.054 | 1.00 47.27 | | | С |
| | | 13569 | C | VAL | | | 58.193 | 22.811 | 72.218 | 1.00 48.65 | | | C |
| | ATOM ATOM | 13570 | | VAL | | | 58.321 | 22.079 | 71.264 | 1.00 52.66 | | • | 0 |
| 50 | | 13571 | N | ARG | | | 57.955 | 22.378 | 73.446 | 1.00 48.25 | | | N |
| 50 | ATOM | | | ARG | | | 57.728 | 20.980 | 73.704 | 1.00 44.23 | . ' | | ·C |
| • | ATOM | 13573 | | ARG | | | 58.145 | 20.582 | 75.105 | 1.00 43.93 | | | Ċ |
| | MOTA | 13575 | | | | | | | 75.427 | 1.00 45.83 | | | С |
| | ATOM | 13578 | CG | ARG | | | 57.739 | | 76.591 | 1.00 44.68 | | | C |
| | ATOM | 13581 | CD | ARG | | | 58.485 | | | | | | N |
| 55 | ATÓM | 13584 | NE | ARG | | | 59.906 | | 76.346 | | | | C |
| | ATOM | 13586 | | ARG | | | 60.516 | | 75.875 | | | | |
| | ATOM | | | 1 ARG | | | 59.848 | | 75.591 | | | | N |
| | ATOM | 13590 | NH | 2 ARG | | | 61.827 | | 75.698 | | | | N |
| | MOTA | 13593 | С | ARG | C 96 | | 56.242 | | 73.546 | | | | C |
| 60 | | | 0 | ARG | C 96 | | 55.491 | | 74.008 | | | | 0 |
| - | ATOM | | N | ALA | | | 55.813 | 19.729 | 72.908 | 1.00 43.97 | • | | N |
| | | • | | | | | | | | | | | |

| | | * | | | | • | | | | | | | | • | | | |
|------|-----------|----------------|--------|------------|-----|------------|---|-----|-------|------------------|--------|------|-------|---|---|---|----|
| 5 | MOTA | 13597 | CA | ALA | Ċ | 97 | | 54. | 388 | 19.518 | 72.622 | | 42.35 | | | | С |
| • | ATOM | 13599 | CB | ALA | C. | 97 | | 54. | 060 | 20.108 | 71.278 | | 42.11 | | | | С |
| | ATOM | 13603 | С | ALA | С | 97 | | 53. | 894 | 18.105 | 72.636 | | 40.41 | | | | С |
| | ATOM | 13604 | 0 | ALA | С | 97 | | 54. | 575 | 17.166 | 72.319 | | 51.69 | | | | 0 |
| | ATOM | 13605 | N | ASN | | 98 | | 52. | 651 | 17.957 | 72.994 | 1.00 | 46.04 | | | | N |
| 10 | ATOM | 13607 | CA | ASN | | 98 | | 52. | 017 | 16.668 | 72.887 | | 44.67 | | | | С |
| 10 | ATOM | 13609 | CB | ASN | | 98 | | 50. | 544 | 16.823 | 73.230 | 1.00 | 44.47 | | | | С |
| | ATOM | 13612 | CG | ASN | | 98 | | 50. | 342 | 17.320 | 74.619 | 1.00 | 44.86 | | | | Ç |
| | ATOM | 13613 | | ASN | | 98 | | | 884 | 16.760 | 75.563 | 1.00 | 46.18 | | | | Ο. |
| | ATOM | 13614 | | ASN | | 98 | | 49. | 564 | 18.378 | 74.762 | 1.00 | 48.48 | | | | Ņ |
| 15 | ATOM | 13617 | C | ASN | | 98 | | | 175 | 16.171 | 71.463 | 1.00 | 41.60 | | | | С |
| IJ | | 13618 | ŏ | ASN | | 98 | | | 201 | 16.957 | 70.538 | 1.00 | 39.27 | | | | 0 |
| | ATOM | 13619 | N | ILE | | .99 | | | 269 | 14.866 | 71.286 | 1.00 | 41.90 | | | | N |
| | ATOM | 13621 | CA | ILE | | 99 | | | 403 | 14.307 | 69.954 | 1.00 | 46.94 | | | | С |
| • | ATOM | 13623 | CB | ILE | | 99 | | | .861 | 14.330 | 69.470 | | 41.20 | | | | С |
| 20 | ATOM | 13625 | | ILE | | 99 | | | 362 | 15.744 | 69.192 | | 46.97 | | | | С |
| 20 | ATOM | 13628 | , | ILE | | 99 | | | .885 | 15.841 | 68.773 | 1.00 | 44.25 | | | | С |
| * | | 13632 | | ILE | | 99 | | | 939 | 13.652 | 68.168 | | 45.91 | | | | C |
| | MOTA | 13636 | C | ILE | | 99 | | | .914 | 12.870 | 69.953 | | 47.27 | | | | Ç |
| | MOTA | 13637 | Ö | ILE | | 99 | | | .407 | 12.081 | 70.711 | | 58.57 | | | | Ó |
| 25 | MOTA | 13638 | N | ALA | | | | | .944 | 12.554 | 69.116 | | 46.89 | | | | N |
| 25 | MOTA | 13640 | CA | ALA | | | | | .418 | 11.219 | 68.962 | | 46.93 | | | | С |
| | ATOM | 13642 | CB | ALA | | | | | .949 | 11.274 | 68.540 | | 45.92 | | | | С |
| | ATOM | | | ALA | | | | | .197 | 10.514 | 67.884 | | 48.45 | | | | С |
| | ATOM | 13646 | C | ALA | | | | | .172 | 10.906 | 66.711 | | 45.06 | | | | 0 |
| 20 | MOTA | 13647 | 0 | ALA | | | | | .872 | 9.436 | 68.250 | | 47.39 | | | | N |
| 30 | MOTA | 13648 | N | ALA | | | | | .639 | 8.732 | 67.260 | | 46.43 | | | | С |
| | ATOM | 13650 | CA | ALA | | | | | .820 | 8.041 | 67.940 | | 47.14 | | | | C |
| | ATOM | 13652 | CB | | | | | | .690 | 7.749 | 66.604 | | 41.79 | | | | Ċ |
| | ATOM | 13656 | , C, | ALA | | | | | :118 | 6.968 | 67.307 | | 48.05 | | | | Ō |
| 25 | ATOM | 13657 | 0 | ALA | | | | | .500 | 7.781 | 65.285 | | 42.66 | | | | N |
| 35 | MOTA | 13658 | N | ILE ILE | | | | | .507 | 6.878 | 64.635 | • | 42.52 | | | | C |
| | ATOM | 13660 | CA | | | 102 | | | .916 | 7.478 | 63.366 | | 37.68 | | | | č |
| | ATOM | 13662 | CB | ILE | | | | | .273 | 8.809 | 63.646 | | 42.95 | | | | C |
| | ATOM | 13664 | | LILE | | | | | .029 | 9.597 | 62.382 | | 48.42 | | , | | С |
| àΩ | ATOM | 13667 | | S IFE | | | | | .845 | 6.590 | 62.789 | | 42.11 | | | | c |
| 40 - | ATOM | 13671 | | | | 102 | | | .141 | 5.609 | 64.183 | | 42.17 | | | | С |
| | ATOM | 13675 13676 | С | | | 102 | | | .146 | 5.671 | 63.469 | | 50.97 | | | | 0 |
| | ATOM | | O N | | | 103 | • | | .529 | 4.493 | 64.581 | | 39.36 | | | | N |
| | ATOM | 13677 | CA | | | 103 | | | .950 | 3,.130 | 64.257 | | 38.74 | | | | С |
| 45 | MOTA | 13679 | CB | | | 103 | | | .024 | 2.324 | 65.542 | | 31.31 | | | | C |
| 40 | MOTA MOTA | 13681 13683 | | 1 THR | | | | | .802 | 2.511 | 66.252 | | 37.91 | | | | 0. |
| • | | 13685 | | 2 THR | | | | | .988 | 2.821 | 66.443 | | 25.93 | | | | С |
| | ATOM | | _ | | | 103 | | | .936 | 2.306 | | | | | | | C. |
| | ATOM | 13689 | C | | | | | | .222 | 1.153 | 63.067 | | 49.83 | | • | | Ο. |
| 50 | ATOM | 13690 | 0 | | | 103 104 | | | .764 | 2.866 | 63.161 | | 50.27 | | | • | N |
| 50 | MOTA | 13691 | | | | | | | .674 | 2.128 | 62.535 | | 52.57 | | | | C |
| | MOTA | 13693 | CA | | | 104 104 | | | .967 | 1.315 | | | 58.34 | | | | Ċ |
| | ATOM | 13695 | CB | | | | | | | -0.048 | 63.935 | | 69.41 | | | | c |
| : | ATOM | 13698 | CG | | | 104 | | | .546 | -0.983 | | | 78.52 | | | | Č |
| | ATOM | 13701 | CD | | | 104 | | | .428 | | | | 80.85 | | | | ŏ |
| 55 | ATOM | 137.02 | OE. | 1 GLU | | 104 | | | .341 | -0.435 -2.229 | | | 82.93 | | | | Ö |
| | ATOM | | | 2 GLU | | | | | 629 | 3.068 | 62.052 | | 48.07 | | | | ,Ċ |
| | ATOM | | C | | | 104 | | | .607 | 3.888 | | | 35.83 | | | | o |
| | ATOM | 13705 | 0 | | | 104 | | | 105 | | | | 49.78 | | | | N |
| 60 | ATOM | | | | | 105 | | | 1.185 | 2.970 | | | 51.92 | | | | C |
| 60 | ATOM | | CA | | | 105 | | | .155 | 3.896 | | | 48.19 | | | | č |
| | ATOM | 13710 | CB | SER | · C | 105 | | 4.5 | .802 | 5.173 | JJ.021 | 00 | 40.13 | • | | • | - |

| 5 | ATOM | 13713 | OG | SER (| C 105 | 4 | 6.446 | 4.896 | 58.587 | 1.00 | 50.41 | | C | |
|-----|------|-------|-----|-------|-------|---|--------|--------|------------------|------|----------------|----|-----|--------|
| | MOTA | 13715 | С | SER (| C 105 | 4 | 4.336 | 3.307 | 59.195 | 1.00 | 53.97 | | C | ; |
| | ATOM | 13716 | 0 | SER (| C 105 | 4 | 4.748 | 2.324 | 58.583 | 1.00 | 54.52 | | C |) |
| | MOTA | 13717 | N | | C 106 | 4 | 3.190 | 3.933 | 58.931 | 1.00 | 48.85 | | N | 1 |
| | ATOM | 13719 | | | C 106 | | 2.327 | 3.568 | 57.825 | 1.00 | 54.43 | | C | ; |
| 10 | ATOM | 13721 | | | C 106 | | 1.117 | 2.695 | 58.274 | 1.00 | 53.40 | | C | 3 |
| 10 | ATOM | 13724 | CG | | 2 106 | | 0.419 | 1.971 | 57.076 | | 59.23 | | (| ; |
| | ATOM | 13725 | | | 2 106 | | 1.164 | 1,374 | 56.243 | | 60.96 | | C | |
| | ATOM | 13726 | | | C 106 | | 9.146 | 1.940 | 56.861 | | 64.74 | | Ċ | |
| | ATOM | 13727 | C C | | C 106 | | 1.882 | 4.891 | 57.127 | | 53.64 | | Ċ | |
| 15 | | | | | C 106 | | 1.304 | 5.783 | 57.734 | | 51.47 | | Č | |
| 13 | MOTA | 13728 | 0 | | C 107 | | 2.204 | 4.992 | 55.848 | | 54.37 | | 1 | |
| | ATOM | 13729 | N | | | | 1.853 | 6.116 | 54.999 | | 51.97 | | | |
| | MOTA | 13731 | | | C 107 | | 0.405 | 5.986 | 54.532 | | 53.57 | | Ò | |
| • | ATOM | 13733 | CB | | C 107 | | | 4.542 | 54.124 | | 55.39 | | Ċ | |
| 20 | ATOM | 13736 | CG | | C 107 | | 9.921 | 4.466 | 54.249 | | 59.86 | | . (| |
| 20 | MOTA | 13739 | CD | | C 107 | | 8.335 | | 53.820 | ~ - | 61.09 | | Ç | |
| | ATOM | 13742 | CE | | C 107 | | 7.629 | 3.148 | | | 53.27 | | | N |
| | MOTA | 13745 | NZ | | C 107 | | 6.060 | 3.234 | 53.879 | | | | | S C |
| | ATOM | 13749 | C | | C 107 | | 2.133 | 7.499 | 55.610 | | 50.56 | | | 5 |
| 0.5 | ATOM | 13750 | 0 | | C 107 | | 1.383 | 8.440 | 55.412 | | 51.18 | | | J N |
| 25 | MOTA | 13751 | N | | C 108 | | 3.223 | 7.613 | | | 48.34 | | | S C |
| | ATOM | 13753 | | | C 108 | | 3.712 | 8.905 | 56.787 | | 47.27 | | | C |
| | ATOM | 13755 | CB | | C 108 | | 4.540 | 8.748 | 58.031 | | 45.62 | | | C |
| | ATOM | 13758 | | | C 108 | | 4.938 | 10.029 | 58.643 | | 37.04 | • | | C |
| 20 | MOTA | 13759 | | | C 108 | | 3.993 | | 59.105 | | 38.32 | | | C |
| 30 | ATOM | 13761 | | | C 108 | | 4.362 | 12.075 | 59.688 | | 40.30 | | | C |
| • | MOTA | 13763 | | | C 108 | | 15.663 | 12.392 | 59.804 | | 33.49 | | | |
| | MOTA | 13765 | | | C 108 | | 16.603 | 11.535 | 59.347 | | 37.53 | • | | C . |
| | MOTA | 13767 | | | C 108 | | 16.237 | 10.357 | 58.770 | | 36.71 | | | C |
| 25 | ATOM | 13769 | С | | C 108 | | 14.660 | 9.440 | 55.747 | | 50.97 | | | 0 |
| 35 | ATOM | 13770 | 0 | | C 108 | | 14.408 | 10.462 | • | | 53.65 | | | N |
| | MOTA | 13771 | N | | C 109 | | 15.768 | 8.718 | | | 47.95 | | | N C |
| | MOTA | 13773 | CA | | C 109 | | 16.805 | 9.096 | 54.701 | | 47.94 | | . (| |
| | MOTA | 13775 | CB | | C 109 | | 18.006 | 8.198 | 54.915 | | 45.29 | | | C |
| 40 | ATOM | 13778 | CG | | C 109 | | 18.678 | 8.429 | 56.255 | | 46.27 48.64 | | | C |
| 40 | MOTA | 13779 | | | C 109 | | 19.046 | 7.389 | 57.063 | | 47.73 | | | C - |
| | ATOM | 13781 | | | C 109 | | 19.637 | 7.618 | 58.276 | | 47.73 | | | C |
| | ATOM | 13783 | CZ | | C 109 | | 19.873 | 8.893 | 58.689 | | 48.66 | | | c. |
| | ATOM | 13785 | | | C 109 | | 19.518 | 9.933 | 57.901 56.698 | | | | | C . |
| AE | ATOM | 13787 | | | C 109 | | 18.922 | 9.707 | | | 49.42 | | | c |
| 45 | MOTA | 13789 | C | | C 109 | | 16.226 | • | | | 53.22 60.08 | | | 0 |
| | ATOM | 13790 | 0 | | C 109 | | 15.213 | 8.362 | 53.118 | | 52.83 | | | N . |
| | ATOM | 13791 | N | | C 110 | | 16.836 | 9.748 | 52.359 | | | | | C. |
| | MOTA | 13793 | CA | | C 110 | | 16.374 | 9.790 | | | | | | - |
| | ATOM | 13795 | CB | | C 110 | | 45.836 | 11.149 | 50.688 | | 53.27 | | | C |
| 50 | ATOM | 13797 | | | C 110 | | 44.566 | | 51.445 | | 52.71 | | | C. |
| | ATOM | 13800 | | | C 110 | | 44.141 | | 51.288 | | 50.55 | | | C |
| | ATOM | 13804 | | | C 110 | | 45.504 | | 49.236 | | 57.99 | | | C - |
| | ATOM | 13808 | C | | C 110 | | 47.519 | | 50.019 | | 54.78 | | | C. |
| | MOTA | 13809 | 0 | | C 110 | | 48.434 | | 49.980 | | 60.18 | | | 0 . |
| 55 | MOTA | 13810 | N | | C 111 | | 47.485 | | 49.227 | | 58.31 | ٠. | | N |
| • | MOTA | 13812 | CA | | C 111 | | 48.617 | | 48.348 | | 58.73 | | | С |
| | ATOM | 13814 | CB | | C 111 | | 48.255 | | 47.389 | | 61.62 | | | C |
| | MOTA | 13817 | CG | | C 111 | | 49.245 | | 46.243 | | 66.55 | | | C |
| · - | MOTA | 13820 | CD | | C 111 | | 48.738 | | | | | | | C: |
| 60 | MOTA | 13821 | | | C 111 | | 49.529 | | 44.450 | | 66.00 | | | 0: |
| | ATOM | 13822 | NE2 | GLN | C 111 | • | 47.415 | 5.837 | 45.099 | 1.00 | 65.39 | • | | N |
| | | | | | | | | | | | | | | |

| | | . | | | | | | | | | | |
|-------|-----------|----------------|----------|-------|----------------|------------------|------------------|------------------|-------|-------|----|--------|
| 5 | ATOM | 13825 | C · | GLN (| C 111 | 49.047 | 9.471 | 47.560 | 1.00 | | • | C |
| | MOTA | 13826 | 0 | GLN (| C 111 | 48.222 | 10.128 | 46.924 | | 57.77 | | 0 |
| | ATOM | 13827 | N | GLY (| C 112 | 50.339 | 9.788 | 47.628 | | 58.53 | | N |
| • | MOTA | 13829 | CA | | C 112 | 50.915 | 10.916 | 46.916 | | 59.25 | | c |
| | ATOM | 13832 | | | C 112 | 50.726 | 12.291 | 47.540 | | 58.52 | | . C |
| 10 | ATOM . | 13833 | 0 | | C 112 | 51.104 | 13.284 | 46.941 | | 54.33 | | 0 |
| | MOTA | 13834 | N | SER (| C 113 | 50.158 | 12.356 | 48.739 | | 59.61 | | N |
| ٠. | MOTA | 13836 | CA | SER (| C 113 | 49.832 | 13.635 | 49.370 | | 59.93 | | C |
| , | MOTA | 13838 | CB | SER (| C 113 | 49.012 | 13.380 | 50.616 | | 61.27 | | C |
| | ATOM | 13841 | OG | SER (| C 113 | 49.791 | 12.666 | 51.583 | | 61.67 | | 0 |
| 15 | MOTA | 13843 | С | | C 113 | 51.044 | 14.401 | 49.826 | 1.00 | | | C |
| | MOTA | 13844 | 0 | SER (| C 113 | 50.970 | 15.560 | 50.136 | | 64.41 | | 0 |
| | MOTA | 13845 | N | | C 114 | 52.168 | 13.730 | 49.879 | 1,.00 | | | N . |
| | MOTA | 13847 | CA | | C 114 | 53.389 | 14.312 | 50.410 | | 58.90 | | C |
| | MOTA | 13849 | CB | | C 114 | 53.911 | 15.426 | 49.496 | 1.00 | | | C |
| 20 | MOTA | 13852 | CĠ | ASN | C 114 | 55.402 | 15.668 | 49.693 | | 62.94 | | . C |
| | MOTA | 13853 | | | C 114 | 56.179 | 14.725 | 49.898 | | 58.01 | • | 0 |
| | ATOM | 13854 | ND2 | | C 114 | 55.807 | 16.931 | 49.657 | | 67.46 | | N |
| | ATOM | 13857 | С | | C 114 | 53.420 | 14.734 | 51.918 | | 52.44 | | C |
| | ATOM | 13858 | .0 | | C 114 | 54.474 | 15.175 | 52.388 | | 53.11 | | 0 |
| 25 | ATOM | 13859 | N | | C 115 | 52.322 | 14.581 | 52.662 | | 48.49 | | N · |
| ₹. | MOTA | 13861 | CA | | C 115 | 52.311 | 14.866 | 54.131 | | 47.90 | | С |
| | ATOM | 138.63 | CB | | C 115 | 51.158 | 15.786 | 54.572 | | 44.85 | | C |
| | ATOM | 13866 | CG | | C 115 | 49.757 | 15.522 | 54.098 | | 35.78 | | C |
| | MOTA | 13867 | CD1 | | C 115 | 49.177 | 16.027 | 52.986 | | 38.12 | | C |
| 30 | MOTA | 13869 | NEl | | C 115 | 47.879 | 15.592 | 52.868 | | 39.72 | | N |
| | MOTA | 13871 | | | C 115 | 47.596 | 14.785 | 53.936 | | 41.98 | | C |
| | MOTA | 13872 | | | C 115 | 48.762 | 14.723 | 54.734 | | 40.24 | | C C |
| | ATOM | 13873 | | | C 115 | 48.733 | 13.947 | 55.898 | | 36.07 | | C |
| 25 | ATOM | 13875 | | | C 115 | 47.597 | 13.286 | 56.223 | | 31.67 | ٠. | . C |
| 35 | ATOM | 13877 | | | C 115 | 46.448 | 13.366 | 55.414 | | 37.70 | | c |
| | ATOM | 13879 | | | C 115 | 46.431 | 14.104 | 54.262 55.024 | | 49.13 | | c |
| | ATOM | 13881 | C | | C 115 | 52.333 | 13.594 12.529 | 54.610 | | 56.05 | | .0 |
| | ATOM | 13882 | 0 | | C 115 C 116 | 51.893 52.835 | 13.694 | 56.246 | | 42.30 | | N |
| 40 | MOTA | 13883 | Ň CZ | | C 116 | 53.060 | 12.493 | 57.029 | | 36.92 | | C |
| 40 | ATOM | 13885 | CA | | C 116 | 54.543 | 12.335 | 57.308 | | 35.88 | | Č |
| | ATOM | 13887 13890 | CB CG | | C 116 | 55.428 | 11.872 | 56.167 | | 40.41 | | Ċ |
| | ATOM | 13893 | ·CD | | C 116 | 56.100 | 12.992 | 55.447 | | 43.69 | | Ċ |
| | MOTA MOTA | 13894 | | | C 116 | 56.149 | 12.999 | 54.197 | | 51.67 | | 0 |
| 45 | ATOM | 13895 | | | C 116 | 56.596 | 13.871 | 56.142 | | 54.68 | | 0 |
| 43 | MOTA | 13896 | C | | C 116 | 52.378 | 12.587 | 58.365 | | 42.27 | | С |
| | ATOM | 13897 | ŏ | | C 116 | 52.608 | 11.744 | 59.249 | ٠. | 44.85 | | 0 |
| | ATOM | 13898 | N | | C 117 | 51.547 | | 58.518 | | 37.85 | | N |
| | ATOM | 13900 | CA | | C 117 | 50.997 | 13.960 | 59.807 | | 33.97 | | С |
| 50 | | 13903 | c . | | C 117 | 50.070 | 15.133 | 59.637 | | 37.13 | | С |
| | ATOM | 13904 | ō | | C 117 | 50.056 | 15.846 | 58.625 | | 35.82 | | 0 |
| | ATOM | 13905 | N | | C 118 | 49.256 | 15.338 | 60.636 | | 36.24 | | N |
| ***** | ATOM | 13907 | CA | | C 118 | 48.332 | 16.425 | 60.572 | 1.00 | 38.55 | | С |
| | ATOM | 13909 | CB | | C 118 | 46.910 | 15.921 | 60:803 | 1.00 | 40.07 | | С |
| 55 | ATOM | 13911 | | | C 118 | 45.865 | 16.999 | 60.568 | 1.00 | 42.31 | | С |
| | ATOM | 13914 | | | C 118 | 44.458 | 16.429 | 60.571 | 1.00 | 40.16 | | , C |
| • | ATOM | 13918 | CG2 | ILE | C 118 | 46.748 | 15.448 | 62.229 | 1.00 | 42.62 | | С |
| • | ATOM | 13922 | С | | C 118 | 48.776 | 17.298 | 61.695 | | 41.59 | | C |
| | ATOM | 13923 | 0 | | C 118. | 49.698 | 16.975 | 62.440 | | 47.04 | | . 0 |
| 60 | ATOM | 13924 | N | LEU | C 119 | 48.111 | 18.419 | 61.807 | | 41.76 | | N |
| | ATOM | 13926 | CA | LEU | C 119 | 48.341 | 19.372 | 62.878 | 1.00 | 39.99 | | С |
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20.360 62.540 1.00 37.22
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    ATOM 13928
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                  CG LEU C 119
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                                                               1.00 35.55
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38.537

39.402

39.507

40.21

3 40.1

3 40.5

23 40.

124 40.

124 40.

124 41.

124 3.

124 3.
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                   CA
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      ATOM
                        ILE C 126
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| | , | | | | | | | | | | | |
|----------------|--------------|----------------|----------|------------------------|---|--------|------------------|------------------|--------------------------|---|-----|--------|
| 5 | ATOM. | 14044 | N | ALA C 127 | | 39.789 | 17.856 | 71.447 | 1.00 44.88 | | | N |
| | MOTA | 14046 | | ALA C 127 | | 41.005 | 17.060 | 71.286 | 1.00 49.29 | | | C |
| * | ATOM | 14048 | CB. | ALA C 127 | | 42.164 | | 71.997 | 1.00 47.42 | | | C |
| | MOTA | 14052 | | ALA C 127 | | 40.708 | 15.676 | 71.871 | 1.00 53.51 | | | С |
| | MOTA | 14053 | 0 | ALA C 127 | • | 39.695 | 15.503 | 72.565 | 1.00 56.30 | | | 0. |
| 10 | ATOM | 14054 | N | ARG C 128 | | 41.570 | 14.700 | 71.591 | 1.00 53.29 | | | -N |
| | MOTA | 14056 | | ARG C 128 | - | 41.396 | 13.345 | 72.102 | 1.00 50.59 | | | C |
| | MOTA | 14058 | CB | ARG C 128 | | 41.159 | 12.348 | | 1.00 57.97 | | • | C |
| | MOTA | 14061 | CG | ARG C 128 | | 39.759 | 12.300 | 70.183 | 1.00 59.94 | | | C |
| | ATOM | 14064 | CD | ARG C 128 | | 38.475 | 12.155 | 71.017 | 1.00 69.66 | | | С |
| 15 | ATOM | 14067 | NE | ARG C 128 | | 37.271 | 12.355 | 70.198 | 1.00 76.55 | | | · N |
| | ATOM | 14069 | CZ | ARG C 128 | | 36.442 | 11.399 | 69.770 | 1.00 84.49 | | | C |
| | MOTA | 14070 | | ARG C 128 | | 36.641 | 10.106 | 70.062 | 1.00 85.61 | | | N |
| | ATOM | 14073 | NH2 | ARG C 128 | | 35.389 | 11.753 | 69.034 | 1.00 86.88 | | | N |
| • | ATOM- | 14076 | С | ARG C 128 | | 42.707 | 13.008 | 72.850 | 1.00 50.92 | | | C |
| 20 | ATOM | 14077 | 0 | ARG C 128 | | 43.799 | | 72.544 | 1.00 47.14 | • | | 0 |
| | MOTA | 14078 | И | PRO C 129 | | 42.662 | | 73.847 | 1.00 45.26 | | | N |
| | MOTA | 14079 | CA | PRO C 129 | | 41.469 | 11.450 | 74.333 | 1.00 42.08 | | | C |
| ٠. | MOTA | 14081 | . CB | PRO C 129 | | 42.028 | 10.478 | 75.365 | 1.00 43.25 | | | C |
| | MOTA | 14084 | ÇG | PRO C 129 | | 43.561 | 10.579 | 75.290 | 1.00 38.09 | | | C |
| 25 | MOTA | 14087 | CD | PRO C 129 | | 43.892 | 11.844 | 74.590 | 1.00 35.38 | | | C |
| | ATOM | 14090 | С | PRO C 129 | | 40.487 | 12.337 | 75.054 | 1.00 49.15 | | | C |
| | ATOM | 14091 | 0 | PRO C 129 | | 39.322 | 11.949 | 75.129 | 1.00 58.20 | | | 0 |
| | MOTA | 14092 | N | ASP C 130 | | 40.919 | 13.483 | 75.578 | 1.00 52.35 | | | N |
| • | MOTA | 14094 | CA · | ASP C 130 | | 40.023 | 14.394 | 76.283 | 1.00 55.40 | | | C |
| 30 | MOTA | 14096 | CB | ASP C 130 | | 39.774 | 13.858 | 77.664 | 1.00 61.87 | | | C |
| | MOTA | 14099 | ÇG | ASP C 130 | | 41.048 | 13.867 | 78.498 | 1.00 70.21 | | | C O |
| | ATOM | 14100 | | ASP C 130 | | 41.533 | 12.794 | 78.934 | 1.00 73.11 | | ' | 0 |
| | MOTA | 14101 | | ASP C 130 | | 41.650 | 14.930 | 78.752 | 1.00 74.28 | | | c |
| | MOTA | 14102 | С | ASP C 130 | | 40.659 | 15.766 | 76.453 | 1.00.55.47 | | | 0 |
| 35 | MOTA | 14103 | 0 | ASP C 130 | | 41.857 | 15.911 | 76.312 | 1.00 47.00 | | | N |
| | MOTA | 14104 | N | ASP C 131 | | 39.835 | 16.755 | 76.804 | 1.00 60.76 1.00 58.88 | | | C |
| | ATOM | 14106 | CA | ASP C 131 | | 40.235 | 18.173 | 76.853 | 1.00 58.88 | | | Ċ |
| | MOTA | 14108 | CB | ASP C 131 | - | 39.051 | 19.107 | 77.223 78.474 | 1.00 03.07 | | | C |
| 40 | ATOM | 14111 | CG | ASP C 131 | | 38.290 | 18.660 17.632 | 79.058 | 1.00 72.14 | | | Ö |
| 40 | MOTA | 14112 | | ASP C 131 | | 38.685 | 19.261 | 78.948 | 1.00 76.88 | • | | ŏ |
| | MOTA | 14113 | | ASP C 131 | | 37.281 | 18.554 | 77.696 | 1.00 70.00 | | | Č |
| | MOTA | 14114 | C. | ASP C 131 | | 41.415 | 19.728 | 77.795 | 1.00 52.31 | - | | Ö |
| • | ATOM | 14115 | 0. | ASP C 131 | | 42.116 | 17.620 | 78.304 | 1.00 47.46 | | | N |
| 45 | MOTA | 14116 | N | SER C 132 SER C 132 | | 43.311 | 17.999 | 79.054 | 1.00 45.98 | | | Ċ. |
| 45 | MOTA | 14118 14120 | CA CB | SER C 132 | | 43.450 | 17.206 | 80.331 | 1.00 46.66 | | | C |
| | ATOM | 14123 | OG | SER C 132 | | 42.859 | 15.924 | 80.195 | 1.00 49.20 | | | 0 |
| | MOTA | 14125 | C | SER C 132 | | 44.574 | 17.843 | | 1.00 47.95 | | | C |
| | ATOM | 14125 | 0 | SER C 132 | | 45.649 | 18.235 | 78.650 | 1.00 52.86 | | | Ō |
| 50 | ATOM | 14127 | N | LEU C 133 | • | 44.449 | 17.292 | 77.015 | | | • | N |
| 30 | ATOM | | CA | LEU C 133 | | 45.591 | 17.140 | 76.156 | 1.00 47.27 | | . • | C |
| | ATOM | 14129 | CB | LEU C 133 | | 45.366 | 16.031 | 75.159 | 1.00 46.70 | | : | C |
| ₁ - | MOTA | 14131 | CG | | | 46.663 | | 74.400 | 1.00 48.65 | | • | · c |
| | MOTA | 14134 14136 | | LEU C 133 | | 47.713 | | 75.385 | | | • | Č |
| 55 | MOTA | | | LEU C 133 | | 46.539 | | | 1.00 50.53 | | | Č |
| 55 | MOTA ATOM | 14140 14144 | CDZ | LEU C 133 | | 45.821 | 18.432 | | 1.00 50.94 | | | Č |
| | ATOM | 14145 | o | LEU C 133 | | 45.405 | | | | | | ō |
| • | ATOM | 14145 | N | GLU C 133 | | 46.478 | | | 1.00 51.70 | | | N |
| | ATOM | 14148 | CA | GLU C 134 | | 46.764 | | | | | | C |
| 60 | ATOM | 14150 | CB | GLU C 134 | | 47.967 | | | | | • | C |
| JU | ATOM | 14153 | CG | GLU C 134 | | 48.225 | | | | | | · c |
| | WIOU | エイエフつ | -00 | 200 C 134 | | | | | | | | - |

| 5 | n moM | 14156 | CD (| GLU C 134 | 49.438 | 23.242 | 76.750 | 1.00 | 65.65 | | | С |
|------------|-------|---------|------|------------|------------|---------|--------|------|---------|---|---|-----|
| 5 | MOTA | | | GLU C 134 | 49.225 | 23.685 | 77.918 | 1.00 | 66.55 | | | 0 |
| | MOTA | 14157 | OE3 | GLU C 134 | 50.605 | 23.183 | 76.240 | | 53.92 | | | 0 |
| | ATOM | 14158 | | | 47.099 | 20.439 | 73.944 | | 55.09 | | | С |
| | MOTA | 14159 | | GLU C 134 | 47.972 | 19.634 | 73.636 | | 51.08 | | | 0 |
| | MOTA | 14160 | | GLU C 134 | | 21.161 | 73.042 | | 52.45 | | | N |
| 10 | MOTA | 14161 | | PRO C 135 | 46.399 | | 71.624 | | 47.35 | | | С |
| | MOTA | 14162 | | PRO C 135 | 46.789 | 21.308 | 71.024 | | 44.20 | | | С |
| | ATOM | | | PRO C 135 | 45.590 | 22.018 | | | 43.96 | | | C. |
| | ATOM | 14167 | | PRO C 135 | 44.524 | 21.918 | 71.952 | | 48.87 | - | | C |
| | ATOM | 14170 | | PRO C 135 | 45.135 | 21.861 | 73.310 | 1 00 | 45.97 | | | Č |
| 15 | MOTA | 14173 | | PRO C 135 | 48.011 | 22.197 | 71.412 | | 57.63 | | | ō |
| | ATOM | 14174 | | PRO C 135 | 48.341 | 23.014. | | | 49.91 | | | N |
| | ATOM | 14175 | | PHE C 136 | 48.665 | 22.030 | 70.271 | | | | | C |
| | ATOM | 14177 | | PHE C 136 | 49.918 | 22.693 | 69.912 | | 41.68 | | | C |
| Ť | MOTA | 14179 | | PHE C 136 | 50.230 | 22.292 | 68.497 | | 41.45 | | | C |
| 20 | MOTA | 14182 | CG | PHE C 136 | 51.358 | 23.034 | 67.882 | | 41.29 | | | |
| .20 | ATOM | 14183 | | PHE C 136 | 52.621 | 22.527 | 67.912 | | 37.45 | | | C |
| | ATOM | 14185 | | PHE C 136 | 53.646 | 23:172 | 67.368 | | 39.54 | | | ·C |
| | MOTA | 14187 | | PHE C 136. | 53.450 | 24.324 | 66.769 | | 46.69 | | | · C |
| | ATOM | 14189 | CE2 | PHE C 136 | 52.202 | 24.861 | 66.706 | | 47.06 | | | C |
| 25 | MOTA | 14191 | | PHE C 136 | 51,152 | 24.216 | 67.266 | 1.00 | 44.15 | | | С |
| 23 | | 14193 | C | PHE C 136 | 49.917 | | 69.976 | 1.00 | 48.49 | | | C. |
| | MOTA | | | PHE C 136 | 50.837 | ٠. | 70.537 | 1.00 | 57.13 | | | 0 |
| | ATOM | 14194 | | PHE C 137 | 48.902 | 24.838 | 69.403 | | 50.04 | | | N |
| | MOTA | 14195 | N | PHE C 137 | 48.879 | 26.300 | 69.407 | 1.00 | 42.38 | | | С |
| án | ATOM | 14197 | | PHE C 137 | 47.751 | 26.868 | 68.559 | | 43.63 | | | С |
| 30 | MOTA | 14199 | CB | | 48.105 | 28.174 | 67.943 | | 44.76 | | | С |
| | MOTA | 14202 | CG | PHE C 137 | 48.912 | 28.224 | 66.849 | | 48.03 | | | С |
| | MOTA | 14203 | | PHE C 137 | 49.260 | 29.420 | 66.290 | | 46.54 | | | С |
| | MOTA | 14205 | | PHE C 137 | 48.814 | 30.560 | 66.820 | | 44.20 | | • | C |
| | MOTA | 14207 | CZ | PHE C 137 | 48.001 | 30.536 | 67.920 | | 43.29 | | | С |
| 35 | MOTA | 14209 | | PHE C 137 | | 29.358 | 68.474 | | 48.04 | | | С |
| | MOTA | 14211 | | PHE C 137 | 47.648 | 26.775 | 70.830 | | 45.85 | | | С |
| | ATOM | 14213 | С | PHE C 137 | 48.782 | 27.784 | 71.210 | | 43.40 | | | 0 |
| | ATOM | 14214 | 0 | PHE C 137 | 49.389 | | 71.651 | | 46.65 | | | N |
| | MOTA | 14215 | N | ASP C 138 | 48.034 | 26.044 | 73.024 | | 48.49 | | | c |
| 40 | MOTA | 14217 | CA | ASP C 138 | 47.918 | 26.481 | | | 50.42 | | | Ċ |
| | MOTA | 14219 | CB | ASP C 138 | 47.010 | | 73.849 | | 56.72 | | | Č |
| | MOTA | 14222 | CG | ASP C 138 | 45.550 | | 73.523 | | 57.59 | | | ŏ |
| | MOTA | 14223 | | ASP C 138 | 44.771 | i | 74.459 | | 63.56 | | | Ö |
| | MOTA | 14224 | OD2 | ASP C 138 | 45.080 | | | | | | | c |
| 45 | ATOM | . 14225 | С | ASP C 138 | 49.321 | | | | 49.79 | | * | ŏ |
| | ATOM | 14226 | 0 | ASP C 138 | 49.664 | | | | 50.18 | | | N |
| | ATOM | 14227 | Ν. | SER C 139 | 50.117 | | | | 45.66 | | | C |
| | MOTA | 14229 | CA | SER C 139 | 51.454 | | 73.832 | | 45.55 | • | | C |
| | ATOM | 14231 | CB | SER C 139 | 52.080 | 23.926 | | | 12.34 | | | |
| 50 | ATOM | | OG | SER C 139 | 51.244 | 22.831 | | | 38.35 | | | 0 |
| , | ATOM | | С | SER C 139 | 52.359 | 26.358 | | | 0 45.80 | | | C |
| | ATOM | | 0 | SER C 139 | 53.036 | 27.041 | 74.081 | | 0 47.40 | | | 0 |
| | ATOM | | N | LEU C 140 | 52.370 | | 72.015 | 1.0 | 0 48.74 | | | N |
| | ATOM | | | LEU C 140 | 53.222 | | 71.365 | | 0 50.72 | | | С |
| 55 | | _ | | LEU C 140 | 52.847 | | | 1.0 | 0 48.34 | | | С |
| 55 | ATOM | | | LEU C 140 | 53.654 | | | | 0 46.32 | | | С |
| | ATOM | | | LEU C 140 | 55.129 | | | | 0 49.60 | | | С |
| | ATOM | | | LEU C 140 | 53.172 | | | | 0 46.89 | | ٠ | С |
| | ATOM | | | LEU C 140 | 53.041 | | | | 0 51.24 | | | C |
| C 0 | ATOM | | | | 53.989 | | | | 0 55.86 | | | 0 |
| 60 | ATOM | | | LEU C 140 | | | | | 0 53.08 | | | N |
| | ATOM | 14257 | N | VAL C 141 | 51.801 | 23.20 | | 1.0 | | | | |

| 5 | ATOM | 14259 | CA | VAL C 141 | | 51.509 | 30.479 | 72.881 | 1.00 50.16 | • | | С |
|-----|--------------|----------------|--------|------------------|---|------------------|--------|---------|------------|---|---|----|
| | MOTA | 14261 | CB | VAL C 141 | | 50.019 | 30.804 | 72.750 | 1.00 51.99 | | | С |
| | MOTA | 14263 | CG1 | VAL C 141 | | 49.547 | 31.794 | 73.812 | 1.00 48.59 | | | С |
| • | MOTA | 14267 | CG2 | VAL C 141 | | 49.751 | 31.368 | 71.362 | 1.00 55.31 | | | С |
| • | MOTA | 14271 | С | VAL C 141 | | 51.899 | 30.512 | 74.324 | 1.00 52.53 | | | С |
| 10 | MOTA | 14272 | 0 | VAL C 141 | | 52.264 | 31.575 | 74.817 | 1.00 56.14 | | | 0 |
| | ATOM | 14273 | N | LYS C 142 | | 51.828 | 29.375 | 75.019 | 1.00 54.25 | | | N |
| | ATOM | 14275 | CA | LYS C 142 | • | 52.179 | 29.360 | 76.439 | 1.00 54.82 | | | C |
| | ATOM | 14277 | CB | LYS C 142 | • | 51.575 | 28.156 | 77.211 | 1.00 59.67 | | | С |
| | ATOM | 14280 | CG | LYS C 142 | | 50.151 | 28.411 | .77.893 | 1.00 63.35 | | | С |
| 15 | ATOM | 14283 | CD | LYS C 142 | | 49.565 | 27.179 | 78.677 | 1.00 63.97 | | | С |
| | ATOM | 14286 | CE | LYS C 142 | | 48.278 | 27.516 | 79.548 | 1.00 68.51 | | | C· |
| | ATOM | 14289 | NZ | LYS C 142 | | 46.914 | 27.549 | 78.885 | 1.00 62.76 | | | N |
| | ATOM | 14293 | С | LYS C 142 | | 53.692 | 29.426 | 76.618 | 1.00 56.79 | | | С |
| | ATOM | 14294 | 0 . | LYS C 142 | | 54.145 | 30.121 | 77.516 | 1.00 63.76 | | | 0 |
| 20 | ATOM | 14295 | N | GLN C 143 | | 54.476 | 28.760 | 75.759 | 1.00 53.91 | • | | N |
| 20 | ATOM | 14297 | CA | GLN C 143 | | 55.943 | 28.662 | 75.943 | 1.00 47.91 | | | С |
| | ATOM | 14299 | СВ | GLN C 143 | | 56.473 | 27.279 | 75.515 | 1.00 45.64 | • | | С |
| | ATOM | 14302 | CG | GLN C 143 | | 55.935 | 26.091 | 76.354 | 1.00 47.12 | | | С |
| | ATOM | 14305 | CD | GLN C 143 | | 56.055 | 24.720 | 75.636 | 1.00 51.24 | | | С |
| 25 | ATOM | 14306 | | GLN C 143 | | 57.100 | 24.396 | 75.047 | 1.00 54.46 | | | 0 |
| 2.5 | ATOM | 14307 | | GLN C 143 | | 54.990 | 23.927 | 75.695 | 1.00 34.83 | | | N |
| | ATOM | 14310 | C | GLN C 143 | | 56.776 | 29.709 | 75.243 | 1.00 49.87 | | | C |
| | ATOM | 14311 | Ö | GLN C 143 | | 58.000 | 29.605 | 75.260 | 1.00 56.15 | | | ō |
| | ATOM | 14312 | N | THR C 144 | | 56.162 | 30.720 | 74.638 | 1.00 53.26 | | | N |
| 30 | ATOM | 14314 | CA | THR C 144 | | 56.945 | 31.754 | 73.943 | 1.00 54.99 | | | C |
| 30 | ATOM | 14314 | CB · | THR C 144 | | 57.314 | 31.208 | 72.592 | 1.00 55.67 | | | Č |
| | ATOM | 14318 | | THR C 144 | | 56.128 | 30.775 | 71.926 | 1.00 57.59 | | | 0 |
| | ATOM | 14320 | | THR C 144 | | 58.014 | 29.924 | 72.739 | 1.00 56.90 | | | С |
| • | ATOM | 14324 | C· | THR C 144 | | 56.173 | 33.090 | 73.808 | 1.00 57.45 | | | C |
| 35 | ATOM | 14325 | | THR C 144 | | 55.095 | 33.229 | 74.379 | 1.00 57.38 | | | ō |
| 55 | ATOM | 14326 | N | HIS C 145 | | 56.689 | 34.072 | 73.066 | 1.00 57.24 | | | N |
| | ATOM | 14328 | | HIS C 145 | | 55.993 | 35.367 | 72.997 | 1.00 59.37 | | | С |
| | ATOM | 14330 | CB | HIS C 145 | | 56.995 | 36.521 | 73.119 | 1.00 62.64 | | | Č |
| | ATOM | 14333 | CG | HIS C 145 | | 57.622 | 36.612 | 74.472 | 1.00 63.89 | | • | Ċ |
| 40 | ATOM | 14334 | | HIS C 145 | | 58.854 | 36.068 | 74.757 | 1.00 61.12 | | | N |
| -10 | ATOM | 14336 | | HIS C 145 | | 59.142 | 36.279 | 76.028 | 1.00 63.96 | | • | C |
| | ATOM | 14338 | | HIS C 145 | | 58.142 | 36.947 | 76.574 | 1.00 67.84 | | | N |
| | ATOM | 14340 | | HIS C 145 | | 57.177 | 37.168 | 75.623 | 1.00 66.24 | | | C |
| | ATOM | 14342 | C | HIS C 145 | | 55.106 | 35.584 | 71.768 | 1.00 60.03 | | | С |
| 45 | ATOM | 14343 | ŏ | HIS C 145 | | 54.617 | 36.702 | 71.531 | 1.00 61.56 | | | 0 |
| .,, | MOTA | 14344 | N | VAL C 146 | | 54.894 | 34.527 | 70.992 | 1.00 55.68 | ٠ | | N |
| | ATOM | 14346 | CA | VAL C 146 | | 54.037 | 34.612 | 69.813 | 1.00 52.16 | | | С |
| | ATOM | 14348 | СВ | VAL C 146 | | 54.067 | 33.241 | 69.003 | 1.00 53.83 | | | C |
| | ATOM | 14350 | | VAL C 14 | | 52.899 | 33.085 | 68.012 | 1.00 49.94 | | | С |
| 50 | ATOM | 14354 | | VAL C 140 | | 55.398 | 33.083 | 68.271 | 1.00 49.83 | | | Ċ |
| 50 | ATOM | 14358 | C | VAL C 140 | | 52.625 | 34.956 | 70.245 | 1.00 41.58 | | | Ċ |
| | MOTA | 14359 | Ö | VAL C 140 | | 52.071 | 34.277 | 71.047 | 1.00 45.36 | | | o |
| | | | N | PRO C 14 | | 52.072 | 36.026 | 69.721 | 1.00 38.73 | | | N |
| | ATOM ATOM | 14360 14361 | CA | PRO C 14 | | 50.672 | 36.434 | 69.934 | 1.00 44.65 | | | C |
| 55 | | | CB | PRO C 14 | | 50.485 | 37.592 | 68.946 | 1.00 47.94 | | • | Č |
| , | MOTA | 14363 | CG | PRO C 14 | | 51.856 | 38.095 | 68.590 | 1.00 47.94 | | | Č |
| | ATOM | 14366 | CD | PRO C 14 | | 52.799 | 36.961 | 68.863 | 1.00 48.22 | | | C |
| | MOTA | 14369 | | | | | 35.353 | 69.590 | 1.00 43.63 | | | C |
| | ATOM | 14372 | C | PRO C 14 | | 49.667 49.987 | 34.428 | 68.854 | 1.00 49.34 | | | o |
| 60 | MOTA | 14373 | O N | PRO C 14 | | | 35.451 | 70.075 | 1.00 49.34 | | | N |
| VV | MOTA | 14374 | N | ASN C 14 | | 48.446 | | 69.982 | | | | C |
| | MOTA | 14376 | CA | ASN C 14 | • | 47.568 | 34.263 | 07.702 | 1.00 43.03 | | | C |

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71.201 1.00 38.71
                                             34.109
                                     46.660
                      ASN C 148
    ATOM 14378
                  CB
                                                             1.00 40.63
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                                     46.009
                                              32.750
                      ASN C 148
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                  CG
    MOTA
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                      LEU C 149
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                                                               1.00 50.04
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                                                              1.00 50.52
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                  CD1 LEU C 149
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15
                                                                                    С
                                                               1.00 54.10
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                  CD2 LEU C 149
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          14401
                                                                                    С
                                                               1.00 45.78
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                                              33.856
    ATOM 14405
                      LEU C 149
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                                                               1.00 48.36
                                                                                     0
                                                      65.101
                                              34:024
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                      LEU C 149
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                                                               1.00 42.18
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          14407
                  N
     MOTA
                                                               1.00 42.43
                                                                                     C
                                                      63.036
                      PHE C 150
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20
     MOTA
          14409
                  CA
                                                               1.00 40.98
                                                                                     C
                                                       62.984
                      PHE C 150
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                                              31.231
     MOTA
           14411
                  CB
                                                               1.00 41.37
                                                                                     С
                                                      63.059
                      PHE C 150
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                  CG
     ATOM
                                                                                     С
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                  CD1 PHE C 150
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                                              29.924
     MOTA
           14415
                                                               1.00 40.05
                                                                                     С
                                                       64.352
                                             29.090
                  CE1 PHE C 150
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     ATOM -
           14417
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                                                                                     ·C
                                                       63.198
                                                               1.00 39.23
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                      PHE C 150
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25
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     ATOM
                                                                                     C
                                                               1.00 32.22
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                                                       61.978
                                     44.615
                  CE2 PHE C 150
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     MOTA
                                                               1.00 32.36
                                                                                     C
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     MOTA
                                                               1.00 43.38
                                                                                     С
                                                       61.950
                      PHE C 150
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                  С
     MOTA
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                      PHE C 150
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                                                                                     N
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                                                               1.00 43.07
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                                              33.329
                       SER C 151
30
           14427
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     MOTA
                                                               1.00 37.49
                                                                                     C
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                      SER C 151
                  CA
     MOTA
           14429
                                                                                     C
                                                       59.423
                                                               1.00 44.33
                                              35.259
                       SER C 151
                                      46.225
                  CB
           14431
     MOTA
                                                                                     0
                                                               1.00 42.06
                                              35.588
                                                       59.289
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                  OG
                     SER C 151
     MOTA
                                                                                     С
                                                               1.00 38.78
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                       SER C 151
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           14436
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                      SER C 151
                                      47.577
                                              32.606
35
           14437
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                       LEU C 152
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           14440
                  CA
                                                                                     C
                                                               1.00 35.95
                                               30.324
                                                       56.518
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     MOTA
                                                               1.00 36.57
                                                                                     C
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                       LEU C 152
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     MOTA
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                   CD1 LEU C 152
40
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           14447
                                                                                     С
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                   CD2 LEU C 152
           14451
     MOTA
                                                                                     С
                                                       55.023
                                                                1.00 41.15
                                               32.288
                       LEU C 152
                                      45.330
           14455
                   С
     MOTA
                                                                                     O
                                     44.319
                                               32.983
                                                       54.936
                                                                1.00 46.18
                       LEU C 152
           14456
                   0
     MOTA
                                                                                     N
                                                                1.00 40.76
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                                               32.001
                                                       54.003
                       GLN C 153
           14457
                   N
     MOTA
                                                                                     C
                                                                1.00 36.05
                                      45.914
                                               32.418
                                                       52.632
                       GLN C 153
45
           14459
                   CA
     MOTA
                                                                                      С
                                                                1.00 39.58
                                      46.847
                                               33.554
                                                       52.203
                       GLN C 153.
           14461
                   CB
     ATOM -
                                                                                      C
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                                                       50.905
                                      46.387
                                               34.255
                       GLN C 153
      MOTA
            14464
                   CG
                                                                                      С
                                                       50.160
                                                                1.00 49.21
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                                               35.042
                       GLN C 153
            14467
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      ATOM
                                                                1.00 61.46
                                                                                      0
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            14468
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                   NE2 GLN C 153
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            14469
     MOTA
                                                                                      C
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      MOTA
                                                                                      0
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                                               30.910
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                                                                1.00 36.48
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      MOTA
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                                                        50.558
                       LEU C 154
      ATOM
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                   CA
                                                                                      С
                                                                1.00 35.94
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      MOTA
                                                                                      C
                                               27.928
                                                                1.00 28.19
                                                        52.434
                                      44.128
                       LEU C 154
            14481
                   CG
      ATOM
                                                                                      С
                                               26.789
                                                        52.499
                                                                1.00 34.51
                                      43.246
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      ATOM
                                                                                      C
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                                               27.455
                                                        52.858
                                                                1.00 41.55
                   CD2 LEU C 154
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      MOTA
                                                                                      С
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                                                                1.00 41.40
                                       45.144
            14491
                        LEU C 154
                   С
      MOTA
                                                                1.00 47.72
                                       44.050
                                               29.970
                                                        48.695
                        LEU C 154
            14492
                   О
      MOTA
                                                        48.214
                                                               1.00 49.18
                                       46.150
                                               29.419
            14493
                       CYS C 155
      MOTA
                   N
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| | | | | | | | | • | | |
|-----|------|-------|-----|-------------|--------|--------|--------|------------|---|------------|
| 5 | ATOM | 14495 | CA | CYS C 155 | 45.953 | 29.761 | 46.804 | 1.00 56.83 | | c |
| - | ATOM | 14497 | CB | CYS C 155 | 47.143 | 30.559 | 46.285 | 1.00 59.70 | | C |
| | ATOM | 14500 | SG | CYS C 155 | 47.453 | 32.045 | 47.258 | 1.00 65.72 | | S |
| | ATOM | 14501 | С | CYS C 155 | 45.685 | 28.565 | 45.895 | 1.00 59.52 | | C |
| | ATOM | 14502 | 0 | CYS C 155 | 46.576 | 27.824 | 45.515 | 1.00 59.33 | | 0 |
| 10 | ATOM | 14503 | N | GLY C 156 | 44.433 | 28.358 | 45.538 | 1.00 66.70 | | N |
| 10 | ATOM | 14505 | CA | GLY C 156 | 44.157 | 27.304 | 44.582 | 1.00 69.05 | | C |
| | MOTA | 14508 | С | GLY C 156 | 44.971 | 27.693 | 43.359 | 1.00 71.96 | | C |
| | ATOM | 14509 | 0 | GLY C 156 | 45.119 | 28.899 | 43.050 | 1.00 71.30 | • | 0 |
| | ATOM | 14510 | N | ALA C 157 | 45.508 | 26.710 | 42.655 | 1.00 71.91 | | N |
| 15 | ATOM | 14512 | CA | ALA C 157 | 46.331 | 27.044 | 41.517 | 1.00 75.82 | | C. |
| : | ATOM | 14514 | CB | ALA C 157 | 47.022 | 25.831 | 40.962 | 1.00 75.63 | | C |
| | MOTA | 14518 | С | ALA C 157 | 45.458 | 27.645 | 40.467 | 1.00 79.16 | | C |
| | ATOM | 14519 | Ō | ALA C 157 | 45.896 | 28.525 | 39.731 | 1.00 85.18 | | 0 |
| | ATOM | 14520 | N | GLY C 158 | 44.215 | 27.185 | 40.402 | 1.00 81.03 | | N |
| 20 | ATOM | 14522 | CA | GLY C 158 | 43.361 | 27.576 | 39.309 | 1.00 82.68 | | С |
| 20. | ATOM | 14525 | C | GLY C 158 | 43.851 | 26.802 | 38.095 | 1.00 86.22 | | С |
| | ATOM | 14526 | ō | GLY C 158 | 43.962 | 27.338 | 36.995 | 1.00 88.16 | | 0 |
| | ATOM | 14527 | N | PHE C 159 | 44.180 | 25.537 | 38.355 | 1.00 89.75 | | N |
| | ATOM | 14529 | CA | PHE C 159 | 44.445 | 24.472 | 37.374 | 1.00 92.50 | | C |
| 25 | ATOM | 14531 | СВ | PHE C 159 | 45.328 | 24.878 | 36.180 | 1.00 92.91 | | С |
| 23 | ATOM | 14534 | CG | PHE C 159 | 46.710 | 25.287 | 36.552 | 1.00 92.61 | | С |
| • | ATOM | 14535 | | PHE C 159 | 46.993 | 26.621 | 36.810 | 1.00 92.40 | | . C |
| | MOTA | 14537 | | PHE C 159 | 48.259 | 27.023 | 37.155 | 1.00 93.74 | | С |
| | ATOM | 14539 | CZ | PHE C 159 | 49.284 | 26.084 | 37.244 | 1.00 96.27 | | С |
| 30 | ATOM | 14541 | | PHE C 159 | 49.017 | 24.741 | 36.984 | 1.00 95.81 | | С |
| 50 | ATOM | 14543 | | PHE C 159 | 47.728 | 24.349 | 36.637 | 1.00 93.97 | | C . |
| | ATOM | 14545 | C | PHE C 159 | 45.035 | 23.300 | 38.180 | 1.00 94.38 | | С |
| | ATOM | | Ö | PHE C 159 | 45.615 | 23.503 | 39.255 | 1.00 93.80 | | 0 |
| | ATOM | 14547 | N | PRO C 160 | 44.868 | 22.076 | 37.689 | 1.00 95.18 | | N |
| 35 | ATOM | 14548 | CA | PRO C 160 | 45.344 | 20.917 | 38.441 | 1.00 96.99 | | С |
| 33 | ATOM | 14550 | CB | PRO C 160 | 44.632 | 19.747 | 37.789 | 1.00 95.07 | | С |
| | ATOM | 14553 | CG | PRO C 160 | 44.282 | 20.215 | 36.425 | 1.00 96.10 | | С |
| | ATOM | 14556 | CD | PRO C 160 | 44.225 | 21.697 | 36.420 | 1.00 94.57 | • | С |
| | ATOM | 14559 | С | PRO C 160 | 46.848 | 20.733 | 38.357 | 1.00101.28 | | С |
| 40 | ATOM | 14560 | ō | PRO C 160 | 47.540 | 21.320 | 37.505 | 1.00104.32 | | 0 |
| •• | MOTA | 14561 | N | LEU C 161 | 47.336 | 19.898 | 39.267 | 1.00100.82 | | N. |
| | ATOM | 14563 | CÁ | LEU C 161 | 48.746 | 19.635 | 39.405 | 1.00 99.81 | | С |
| | ATOM | 14565 | CB | LEU C 161 | 49.268 | 20.480 | 40.590 | 1.00100.38 | | С |
| | ATOM | 14568 | ĆG | LEU C 161 | 48.819 | 21.960 | 40.588 | 1.00 99.66 | | С |
| 45 | ATOM | 14570 | CD1 | L LEU C 161 | 48.883 | 22.650 | 41.957 | 1.00 99.34 | | C |
| | ATOM | 14574 | CD2 | LEU C 161 | 49.626 | 22.753 | 39.569 | 1.00100.10 | • | C |
| | ATOM | 14578 | С | LEU C 161 | 48.937 | 18.131 | 39.659 | 1.00 98.91 | | С |
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                                      35.698
                                               26.191
                                                       67.216
                                                                1.00 46.95
                                                                                      O
     MOTA
                   0
                                                                                      N
           15157
                       TYR C 199
                                      36.058
                                               26.049
                                                       65.035
                                                                1.00 44.07
     MOTA
                   N
           15159
                                      36.047
                                               27.504
                                                       64.759
                                                                1.00 42.83
     MOTA
                   CA
                       TYR C 199
                                      37.161
                                               27.933
                                                       63.758
                                                                1.00 39.32
60
     MOTA
           15161
                   CB
                       TYR C 199
                                      38.494
                                               28.044
                                                       64.448 1.00 37.70
           15164
     MOTA
                   CG
                       TYR C 199
```

| | | 1 | | | | | | | | | _ |
|------|------|----------------|-----|--------|-----|------------------|----------------------|--------|------------|-----|-----|
| 5 | ATOM | 15165 | | TYR C | | 39.421 | 27.041 | 64.346 | 1.00 40.50 | | C |
| | ATOM | 15167 | CE1 | TYR C | 199 | 40.637 | 27.114 | 65.007 | 1.00 42.66 | | . C |
| | ATOM | 15169 | CZ | TYR C | 199 | 40.932 | 28.211 | 65.793 | 1.00 44.12 | | C |
| | ATOM | 15170 | OH | TYR C | 199 | 42.147 | 28.239 | 66.426 | 1.00 35.21 | | 0 |
| | ATOM | 15172 | CE2 | TYR C | 199 | 40.008 | 29.247 | 65.931 | 1.00 37.43 | | C |
| 10 | ATOM | 15174 | CD2 | TYR C | 199 | 38.800 | 29.152 | 65.263 | 1.00 40.32 | | C |
| | ATOM | 15176 | С | TYR C | 199 | 34.647 | 27.733 | 64.200 | 1.00 46.28 | | С |
| | ATOM | 15177 | 0 | TYR C | 199 | 34.443 | 27 ⁻ .731 | 62.985 | 1.00 45.68 | | 0 |
| | ATOM | 15178 | N | GLU C | 200 | 33.685 | 27.902 | 65.104 | 1.00 48.83 | | N |
| | ATOM | 15180 | | GLU C | 200 | 32.273 | 27.958 | 64.746 | 1.00 49.81 | | С |
| 15 | ATOM | 15182 | | GLU C | 200 | . 31.387 | 27.454 | 65.917 | 1.00 51.32 | | С |
| 13 | ATOM | 15185 | | GLU C | | 29.895 | 27.584 | 65.613 | 1.00 55.33 | | С |
| | ATOM | 15188 | | GLU C | | 28.906 | 26.930 | 66.581 | 1.00 53.36 | | С |
| | ATOM | 15189 | | GLU C | | 29.287 | 26.452 | 67.656 | 1.00 54.60 | | 0 |
| • | ATOM | 15190 | | GLU C | | 27.691 | 26.914 | 66.248 | 1.00 53.86 | • | 0 |
| . 20 | ATOM | 15191 | | GLU C | | 31.860 | 29.363 | 64.350 | 1.00 51.65 | | С |
| . 20 | ATOM | 15192 | | GLU C | | 32.292 | 30.315 | 64.973 | 1.00 50.64 | | 0 |
| | ATOM | 15193 | | VAL C | | 31.026 | 29.467 | 63.307 | 1.00 51.45 | | N |
| | | 15195 | | VAL C | | 30.461 | 30.724 | 62.832 | 1.00 46.63 | | · c |
| | MOTA | 15197 | | VAL C | | 31.231 | 31.274 | 61.575 | 1.00 46.72 | | C |
| . 25 | | 15197 | | VAL C | | 32.720 | 31.290 | 61.826 | 1.00 46.42 | | C C |
| 25 | ATOM | | | VAL C | | 30.925 | 30.490 | 60.319 | 1.00 43.26 | | c · |
| | MOTA | 15203 15207 | CGZ | VAL C | | 28.940 | 30.649 | 62.528 | 1.00 44.99 | | С |
| | MOTA | | | VAL C | | 28.376 | 29.572 | 62.414 | 1.00 54.23 | | 0 |
| | MOTA | 15208 | 0 | ILE C | | 28.293 | 31.822 | 62.411 | 1.00 48.31 | | N |
| 20 | MOTA | 15209 | N | ILE C | | 26.856 | 31.919 | 62.056 | 1.00 42.18 | | С |
| 30 | ATOM | 15211 | CA | | | 25.960 | 32.584 | 63.153 | 1.00 46.13 | | C |
| | ATOM | 15213 | CB | ILE C | | 25.705 | 31.620 | 64.319 | 1.00 52.03 | | C |
| | ATOM | 15215 | | ILE C | | 25.703 | 32.297 | 65.708 | 1.00 47.21 | • | Ċ |
| | MOTA | 15218 | | ILE C | | 24.579 | 32.776 | 62.594 | 1.00 47.93 | | C |
| 25 | MOTA | 15222 | | ILE C | | 26.593 | 32.612 | 60.710 | 1.00 43.46 | | ,c |
| 35 | MOTA | 15226 | C | ILE C | | 26.878 | 33.802 | 60.543 | 1.00 38.75 | | Ō |
| • | MOTA | 15227 | 0 . | ILE C | | | 31.835 | 59.782 | 1.00 42.36 | | N · |
| | MOTA | 15228 | N | ILE C | | 26.020 | 32.266 | 58.452 | 1.00 38.42 | | C |
| | MOTA | 15230 | CA | ILE C | | 25.653 | 31.121 | 57.521 | 1.00 30.12 | | Ċ |
| 40 | MOTA | 15232 | CB | | 203 | 25.821 27.291 | 30.844 | 57.270 | | | č |
| 40 | ATOM | 15234 | | ILE C | | , | 29.632 | 56.433 | 1.00 33.30 | | Ċ |
| | MOTA | 15237 | | ILE .C | | 27.493 | 31.425 | 56.216 | 1.00 43.76 | | č |
| | ATOM | 15241 | | ILE C | | 25.129 | 32.651 | 58.419 | 1.00 45.70 | | Č |
| | MOTA | 15245 | C | ILE C | | 24.172 | 31.774 | | 1.00 42.94 | | ō |
| | ATOM | 15246 | 0 | ILE C | | 23.325 | 33.938 | 58.150 | 1.00 42.34 | | N |
| 45 | ATOM | 15247 | N | VAL C | | 23.882 | 34.494 | 58.261 | 1.00 40.88 | | C |
| | ATOM | 15249 | CA | VAL C | | 22.544 | 35.857 | 58.956 | 1.00 39.68 | | · Č |
| • | ATOM | 15251 | СВ | VAL C | | 22.551 | | 60.252 | 1.00 39.60 | | c |
| | MOTA | 15253 | | VAL C | | 23.310 | 35.782 | | | | č |
| | MOTA | 15257 | | VAL C | | 23.163 | | 58.094 | 1.00 38.86 | | C |
| 50 | MOTA | 15261 | G, | VAL C | | 21.836 | | 56.947 | 1.00 41.55 | | 0 |
| | ATOM | 15262 | 0 | VAL C | | 20.631 | | 56.901 | 1.00 40.27 | | N |
| _ | ATOM | 15263 | N | ·ARG C | | 22.546 | | 55.851 | 1.00 44.70 | | |
| | MOTA | 15265 | CA | ARG (| | 21.813 | | 54.594 | 1.00 43.15 | | ·C |
| | MOTA | 15267 | CB | ARG (| | 21.363 | | 54.387 | 1.00 42.20 | | C |
| 55 | ATOM | 15270 | CG | ARG (| | 20.722 | | 53.055 | 1.00 45.65 | | C |
| | MOTA | 15273 | CD | | 205 | 20.529 | | 52.808 | | | C |
| | ATOM | 15276 | NE | | 205 | 20.356 | | 51.406 | | | N |
| • | ATOM | 15278 | CZ | | 205 | 19.209 | | 50.860 | | | C |
| | MOTA | 15279 | NHl | ARG (| 205 | 18.138 | | | | | N |
| 60 | ATOM | | | ARG (| 205 | 19.131 | | | | | N |
| | ATOM | | .c | ARG (| 205 | 22.634 | 34.130 | 53.409 | 1.00 42.48 | 3 · | C |
| | | | | | | | | | | | |

| 5 | ATOM | 15286 | Ο. | ARG C. 205 | | 23.813 | 34.449 | 53.284 | | 41.99 | | | 0 |
|-----|------|---------|-----|-------------|---|----------|--------|--------|------|---------|---|-----|----------------|
| . • | ATOM | 15287 | N | VAL C 206 | | 22.026 | 33.317 | 52.550 | | 40.52 | | | N |
| | ATOM | 15289 | CA | VAL C 206 | | 22.737 | 32.791 | 51.379 | 1.00 | 41.02 | | | С |
| | ATOM | 15291 | СВ | VAL C 206 | | 22.927 | 31.279 | 51.471 | | 40.59 | | | С |
| | ATOM | 15293 | | VAL C 206 | | 23.317 | 30.696 | 50.129 | | 42.15 | | | C |
| 10 | ATOM | 15297 | | VAL C 206 | | 24.031 | 30.961 | 52.462 | | 41.87 | | | С |
| 10 | ATOM | 15301 | С | VAL C 206 | | 22.034 | 33.153 | 50.075 | | 43.12 | | | С |
| | ATOM | 15302 | Ō | VAL C 206 | | 20.813 | 33.046 | 49.996 | 1.00 | 47.55 | | | O _. |
| | ATOM | 15303 | N | GLU C 207 | | 22.806 | 33.595 | 49.065 | 1.00 | 44.82 | | | N |
| | ATOM | 15305 | CA | GLU C 207 | | 22.279 | 34.018 | 47.753 | 1.00 | 41.44 | | | С |
| 15 | ATOM | 15307 | CB | GLU C 207 | | 22.430 | 35.512 | 47.568 | | 41.47 | | | С |
| 1,5 | ATOM | 15310 | CG | GLU C 207 | | 21.512 | 36.430 | 48.314 | 1.00 | 42.60 | | | C |
| | ATOM | 15313 | CD | GLU C 207 | | 22.035 | 37.856 | 48.249 | | 50.19 | | | C |
| | ATOM | 15314 | | GLU C 207 | | 22.821 | 38.160 | 47.296 | | 52.39 | | | 0 |
| • | ATOM | 15315 | | GLU C 207 | | 21.679 | 38.666 | 49.147 | | 46.64 | | | 0 |
| 20 | ATOM | 15316 | c | GLU C 207 | | 23.034 | 33.399 | 46.566 | 1.00 | 41.75 | | | С |
| 20 | ATOM | 15317 | ŏ | GLU C 207 | | 24.211 | 33.080 | 46.689 | 1.00 | 36.68 | | | 0 |
| | ATOM | 15318 | N | ILE C 208 | | 22.342 | 33.253 | 45.423 | | 40.80 | | | N |
| | MOTA | 15320 | CA | ILE C 208 | | . 22.905 | 32.702 | 44.200 | | 40.34 | • | | С |
| | ATOM | 15322 | СВ | ILE C 208 | | 22.245 | 31.408 | 43.864 | | 39.20 | | | С |
| 25 | MOTA | 15324 | | ILE C 208 | | 22.071 | 30.557 | 45.096 | 1.00 | 40.09 | | | С |
| 23 | ATOM | 15327 | | ILE C 208 | | 23.285 | 29.762 | 45.470 | | 40.99 | | • | C |
| | ATOM | 15331 | | ILE C 208 | | 23.075 | 30.663 | 42.809 | | 43.38 | | | С |
| | ATOM | 15335 | C | ILE C 208 | | 22.593 | 33.697 | 43.111 | | 42.32 | | | C. |
| | ATOM | 15336 | ō | ILE C 208 | | 21.440 | 33.839 | 42.734 | 1.00 | 52.77 | • | | О |
| .30 | ATOM | 15337 | N. | ASN C 209 | | 23.622 | 34.358 | 42.581 | 1.00 | 46.89 | | | N |
| 50 | ATOM | 15339 | CA | ASN C 209 | | 23.490 | 35.589 | 41.739 | 1.00 | 39.83 | | | С |
| | ATOM | 15341 | CB | ASN C 209 | | 23.200 | 35.302 | 40.256 | | 34.52 | | | С |
| | ATOM | 15344 | CG | ASN C 209 | | 24.501 | 35.018 | 39.447 | | 36.76 | | | С |
| | ATOM | 15345 | | ASN C 209 | • | 25.573 | 35.001 | 40.006 | | 41.74 | | | 0 |
| 35 | ATOM | 15346 | | ASN C 209 | | 24.391 | 34.808 | 38.132 | 1.00 | 39.00 | | | N |
| - | MOTA | 15349 | С | ASN C 209 | | 22.527 | 36.598 | 42.359 | | 37.58 | | | С |
| | ATOM | 15350 | 0 | ASN C 209 | | 21.701 | 37.132 | 41.701 | | 48.40 | | | 0 |
| | ATOM | 15351 | N | GLY C 210 | | 22.673 | 36.854 | 43.652 | | 46.50 | | | N |
| | ATOM | 15353 | CA | GLY C 210 | | 21.882 | 37.848 | 44.370 | | 41.31 | | | С |
| 40 | ATOM | 15356 | С | GLY C 210 | | 20.518 | 37.398 | 44.884 | | 41.24 | | | С |
| | ATOM | 15357 | 0 | GLY C 210 | | 19.844 | 38.161 | 45.549 | | 37.25 | | | 0 |
| | ATOM | 15358 | N | GLN C 211 | | 20.113 | 36.163 | 44.594 | | 46.35 | | | N |
| | MOTA | 15360 | CA | GLN C 211 | | 18.781 | 35.675 | 44.963 | | 45.47 | * | | C |
| | ATOM | 15362 | CB | GLN C 211 | | 18.262 | 34.732 | 43.882 | | 49.01 | | | C |
| 45 | ATOM | 15365 | CG | GLN C 211 | | 16.792 | 34.340 | 44.050 | | 48.53 | | | C |
| | ATOM | 15368 | CD | GLN C 211 | | 16.314 | 33.366 | 42.969 | • | 52.21 | | | C |
| | ATOM | 15369 | OE | L GLN C 211 | | 17.113 | 32.799 | 42.237 | | 59.52 | | | . 0 |
| | ATOM | 15370 | NE | 2 GLN C 211 | • | 15.007 | | | | 62.94 | | | N |
| | ATOM | 15373 | С | GLN C 211 | | 18.784 | 34.920 | 46.237 | | 44.55 | | • | C |
| 50 | ATOM | 15374 | 0 | GLN C 211 | | 19.593 | 34.039 | 46.396 | | 47.96 | | | .0 |
| | ATOM | 15375 | N | ASP C 212 | | 17.866 | 35.263 | 47.137 | | 47.82 | | . • | N |
| | MOTA | 15377 | CA | ASP C 212 | | 17.721 | 34.610 | 48.445 | | 0 48.03 | • | | C |
| | ATOM | 15379 | CB | ASP C 212 | | 16.568 | 35.289 | 49.184 | | 0 46.60 | | | C |
| | ATOM | 15382 | CG | ASP C 212 | | 16.680 | 35.212 | 50.710 | | 0 54.20 | | | C |
| 55 | MOTA | | | 1 ASP C 212 | | 17.374 | 34.336 | 51.273 | | 0 61.39 | | | 0 |
| | MOTA | 15384 | OD: | 2 ASP C 212 | | 16.077 | 36.007 | 51.457 | | 0 60.59 | | | 0 |
| | ATOM | | | ASP C 212 | | 17.410 | 33.100 | 48.296 | | 0 52.45 | | • | C |
| | ATOM | | 0 | ASP C 212 | | 16.578 | 32.729 | 47.490 | | 0 56.67 | | | O N |
| | ATOM | | N | LEU C 213 | | 18.087 | 32.240 | 49.055 | | 0 55.42 | | | N |
| 60 | ATOM | | | | | 17.742 | | | | 0 56.97 | | | Ç |
| | | · 15391 | CB | LEU C 213 | | 18.895 | 30.033 | 49.754 | 1.0 | 0 58.95 | | | C |
| | | | | | | | | | | | • | | |

| 5 | ATOM | 15394 | CG | LEU C 21 | 13 | 19.416 | 28.788 | 49.047 | | 59.16 | | | С |
|------|--------------|--------------------|----------|-----------|-----|--------|--------|--------|------|---------|-----|---|----|
| • | ATOM | 15396 | | LEU C 23 | 13 | 20.101 | 29.126 | 47.742 | | 63.01 | | | С |
| | ATOM | 15400 | | LEU C 21 | | 20.399 | 28.127 | 49.943 | | 60.50 | | | С |
| | ATOM | 15404 | С | LEU C 21 | 1.3 | 16.458 | 30.806 | 50.017 | | 62.07 | | | С |
| | ATOM | 15405 | 0 | LEU C 23 | | 15.551 | 29.957 | 49.888 | | 61.04 | | | 0 |
| 10 | ATOM | 15406 | N | LYS C 2 | | 16.396 | 31.769 | 50.929 | 1.00 | 63.07 | | | N |
| 10 | ATOM | 15408 | CA | LYS C 2 | | 15.125 | 32.134 | 51.531 | | 65.72 | | | С |
| | ATOM | 15410 | CB | LYS C 2 | | 14.086 | 32.338 | 50.413 | 1.00 | 68.54 | | | C |
| | ATOM | 15413 | CG | LYS C 2 | | 13.163 | 33.531 | 50.668 | 1.00 | 73.60 | | | С |
| | ATOM | 15416 [.] | CD | LYS C 2 | | 11.780 | 33.375 | 50.049 | | 77.37 | | | С |
| 15 | ATOM | 15419 | CE | LYS C 2 | | 10.778 | 34.279 | 50.782 | | 80.25 | | | С |
| 13 | ATOM | 15422 | NZ | LYS C 2 | | 9.511 | 34.543 | 49.997 | 1.00 | 81.27 | | | N |
| | ATOM | 15426 | C | LYS C 2 | | 14.595 | 31.119 | 52.502 | 1.00 | 65.65 | | | С |
| | ATOM | 15427 | ŏ | LYS C 2 | | 13.379 | 30.934 | 52.638 | 1.00 | 66.01 | | | 0 |
| | ATOM | 15428 | N | MET C 2 | | 15.509 | 30.463 | 53.188 | 1.00 | 63.58 | • | | N |
| 20 | ATOM | 15430 | CA | MET C 2 | | 15.135 | 29.471 | 54.158 | 1.00 | 61.94 | | | C |
| . 20 | ATOM | 15432 | CB | MET C 2 | | 16.070 | 28.284 | 53.990 | 1.00 | 61.98 | • | | С |
| | | 15435 | CG | MET C 2 | | 15.962 | 27.721 | 52.571 | 1.00 | 65.30 | | | С |
| | MOTA | 15438 | SD | MET C 2 | | 17.057 | 26.390 | | | 66.94 | | | S |
| | ATOM | | CE | MET C 2 | | 17.630 | 26.053 | 53.654 | | 69.99 | | | С, |
| 25 | ATOM | 15439 | | MET C 2 | | 15.206 | 30.067 | 55.558 | | 61.53 | | | C |
| 25 | ATOM | 15443 | C | MET C 2 | | 15.628 | 31.208 | 55.733 | | 62.98 | | | 0 |
| | ATOM | 15444 | O N | ASP C 2 | | 14.770 | 29.312 | 56.552 | | 59.98 | • | | N |
| | ATOM | 15445 | | ASP C 2 | | 14.984 | 29.732 | 57.917 | | 63.83 | | | С |
| • | ATOM | 15447 | CA CB | ASP C 2 | | 14.421 | 28.723 | 58.910 | | 63.59 | | | C |
| 20 | MOTA | 15449 | CG | ASP C 2 | | 14.491 | 29.219 | 60.341 | | 63.16 | | | C |
| 30 | MOTA | 15452 | | ASP C 2 | | 15.548 | 29.759 | 60.739 | | 69.24 | | | 0 |
| | MOTA | 15453 | | ASP C 2 | | 13.541 | 29.119 | | | 58.32 | | | 0 |
| | ATOM | 15454 | | ASP C 2 | | 16.489 | 29.813 | 58.110 | | 67.41 | | | С |
| | ATOM | 15455 | С | ASP C 2 | | 17.241 | 28.950 | 57.662 | | 70.90 | | | 0 |
| 25 | ATOM | 15456 | 0 | CYS C 2 | | 16.938 | 30.845 | 58.787 | | 68.15 | | | N |
| 35 | ATOM | 15457 | N | CYS C 2 | | 18.351 | 31.024 | 58.969 | | 72.70 | | | C |
| • | ATOM | 15459 | CA CB | CYS C 2 | | 18.529 | 32.328 | 59.712 | | 74.24 | | | .C |
| | ATOM | 15461 | SG | CYS C 2 | | 18.246 | 32.242 | 61.449 | | 86.77 | | | S |
| | ATOM | 15464 | C | CYS C 2 | | 19.059 | 29.819 | 59.668 | | 71.10 | | | С |
| 40 | ATOM | 15465 | | CYS C 2 | | | 29.351 | 59.235 | | 66.77 | | • | 0 |
| 40 | ATOM | 15466 | O N | LYS C 2 | | 18.447 | 29.314 | 60.736 | | 70.12 | | | N. |
| | ATOM ATOM | 15467 15469 | CA | LYS C 2 | | 18.971 | 28.156 | 61.466 | | 67.64 | | | C |
| | | 15471 | CB | LYS C 2 | | 17.922 | 27.688 | 62.483 | | 67.20 | | | C |
| | ATOM | 15474 | CG | LYS C 2 | | 17.853 | 28.475 | 63.795 | | 70.89 | | | С |
| 45 | ATOM | 15477 | CD | LYS C 2 | | 17.000 | 27.722 | 64.838 | | 73.15 | • | | С |
| 43 | MOTA | 15480 | CE | LYS C 2 | | 16.593 | 28.602 | | | 74.74 | | | С |
| | ATOM | 15483 | NZ | LYS C 2 | | 15.949 | 29.917 | 65.624 | | 73.64 | | | N |
| | MOTA | | _ | LYS C 2 | | 19.318 | 26.997 | | | 63.47 | | | C |
| | ATOM | 15487 | C | | | 20.271 | 26.234 | 60.716 | | 60.95 | | | 0 |
| 50 | ATOM | 15488 | 0 | LYS C 2 | | 18.540 | 26.865 | 59.462 | | 60.07 | | | N |
| 50 | ATOM | 15489 | N | | | 18.752 | 25.751 | 58.582 | | 60.47 | | | С |
| | ATOM | 15491 | CA | GLU C | | 17.606 | 25.606 | 57.552 | | 61.66 | | • | С |
| | ATOM | | CB | GLU C | | 16.924 | 24.226 | 57.549 | | 68.73 | | | C- |
| | MOTA | | CG | | | 15.776 | | 58.574 | | 79.28 | | • | С |
| 55 | ATOM | | CD | GLU C | | 14.678 | | 58.418 | | 80.66 | | | ō |
| 55 | MOTA | | | L GLU C : | | 15.962 | | 59.549 | | 81.82 | | | ō |
| | ATOM | | | | | 20.130 | | 57.963 | | 56.72 | | | Ċ |
| • | MOTA | | | GLU C | | 20.130 | | | | 59.58 | | | ō |
| | MOTA | | | GLU C | | 20.748 | | | | 56.94 | | | N |
| ۲۵ | MOTA | | | TYR C | | 22.003 | | | | 51.25 | | | C |
| - 60 | ATOM | | | TYR C | | 22.231 | | | | 50.12 | . • | | ·C |
| | MOTA | 15508 | CB | TYR C | 22U | 22.231 | 20.003 | 30.300 | 1.00 | 5 50.12 | | | _ |

| | | | | | | | | | • | |
|----|-------|-------|-----|---------|-------|--------|--------|--------|------------|-----|
| 5 | MOTA | 15511 | CG | TYR C | 220 · | 21.253 | 29.350 | 55.891 | 1.00 51.08 | С |
| | ATOM | 15512 | CD1 | TYR C | 220 | 20.657 | 30.589 | 56.072 | 1.00 52.25 | C |
| | ATOM | 15514 | CE1 | TYR C | 220 | 19.758 | 31.101 | 55.142 | 1.00 50.67 | C |
| | ATOM | 15516 | CZ | TYR C | 220 | 19.460 | 30.362 | 54.028 | 1.00 48.80 | С |
| | ATOM | 15517 | ОН | TYR C | 220 | 18.584 | 30.861 | 53.123 | 1.00 54.70 | . 0 |
| 10 | ATOM | 15519 | CE2 | TYR C | 220 | 20.029 | 29.140 | 53.811 | 1.00 47.32 | С |
| 10 | ATOM | 15521 | | TYR C | | 20.927 | 28.634 | 54.741 | 1.00 53.35 | С |
| | ATOM | 15523 | C | TYR C | | 23.106 | 26.890 | 58.295 | 1.00 50.69 | С |
| | ATOM | 15524 | ō | TYR C | | 24.252 | 26.689 | 57.913 | 1.00 49.00 | 0 |
| | ATOM | 15525 | N | ASN C | | 22.780 | 26.754 | 59.569 | 1.00 50.57 | N |
| 15 | ATOM | 15527 | CA | ASN C | | 23.770 | 26.262 | 60.506 | 1.00 55.15 | Ċ |
| 13 | ATOM | 15529 | CB | ASN C | | 24.208 | 27.421 | 61.384 | 1.00 55.72 | č |
| | | | CG | ASN C | | 24.244 | 28.687 | 60.624 | 1.00 58.30 | · c |
| | ATOM | 15532 | | | | 25.274 | 29.062 | 60.045 | 1.00 50.30 | |
| • | ATOM | 15533 | | ASN C | | | | | 1.00 60.35 | . N |
| άn | ATOM | 15534 | | ASN C | | 23.104 | 29.357 | 60.582 | 1.00 55.63 | C |
| 20 | ATOM | | , C | ASN C | | 23.219 | 25.081 | 61.310 | | |
| | MOTA | 15538 | 0 | ASN C | | 23.444 | 24.978 | 62.517 | 1.00 53.22 | 0 |
| | MOTA | 15539 | N | TYR C | | 22.510 | 24.188 | 60.627 | 1.00 55.35 | N |
| | MOTA | 15541 | CA | TYR C | | 21.764 | 23.173 | 61.334 | 1.00 55.70 | Ċ |
| | ATOM | 15543 | CB | TYR C | | 20.643 | 22.579 | 60.521 | 1.00 59.55 | C |
| 25 | MOTA | 15546 | CG | TYR C | | 20.139 | 21.358 | 61.212 | 1.00 63.51 | C |
| | MOTA | 15547 | | TYR C | | 19.875 | 21.375 | 62.578 | 1.00 65.98 | C |
| | ATOM | 15549 | | TYR C | | 19.414 | 20.235 | 63.230 | 1.00 69.85 | C |
| | MOTA | 15551 | CZ | TYR C | | 19.215 | 19.049 | 62.511 | 1.00 72.74 | С |
| | MOTA | 15552 | ОН | TYR C | | 18.757 | 17.898 | 63.130 | 1.00 71.88 | 0 |
| 30 | MOTA | 15554 | CE2 | TYR C | 222 | 19.476 | 19.019 | 61.155 | 1.00 72.46 | |
| | MOTA | 15556 | CD2 | TYR C | | 19.940 | 20.174 | 60.515 | 1.00 66.13 | |
| | ATOM | 15558 | С | TYR C | | 22.748 | 22.140 | 61.714 | 1.00 55.15 | |
| | ATOM. | 15559 | 0 | | 222 | 23.304 | 21.468 | 60.853 | 1.00 51.38 | |
| | MOTA | 15560 | N | ASP C | | 22.904 | 22.013 | 63.027 | 1.00 60.19 | |
| 35 | MOTA | 15562 | CA | ASP C | | 24.044 | 21.398 | 63.668 | 1.00 57.35 | |
| | MOTA | 15564 | CB | ASP C | | 24.600 | 20.222 | 62.885 | 1.00 64.20 | |
| | MOTA | 15567 | CG | ASP C | | 25.633 | 19.430 | 63.682 | 1.00 68.05 | |
| | MOTA | 15568 | | ASP C | | 26.491 | 18.782 | 63.058 | 1.00 75.23 | |
| | MOTA | 15569 | OD2 | ASP C | 223 | 25.669 | 19.410 | 64.935 | 1.00 65.90 | |
| 40 | MOTA | 15570 | С | ASP C | | 25.109 | 22.491 | 63.857 | 1.00 53.89 | |
| | MOTA | 15571 | 0 | ASP C | | 25.364 | 22.902 | 64.969 | 1.00 51.49 | |
| | ATOM | 15572 | N | LYS C | | 25.729 | 22.980 | 62.788 | 1.00 51.65 | |
| | ATOM | 15574 | CA | LYS C | 224 | 26.750 | 24.020 | 62.949 | 1.00 48.28 | |
| | MOTA | 15576 | CB | LYS C | | 27.919 | 23.538 | 63.825 | 1.00 49.33 | |
| 45 | MOTA | 15579 | CG | LYS C | | 28.786 | 22.456 | 63.125 | 1.00 50.13 | |
| ** | MOTA | 15582 | CD | LYS · C | | 29.770 | 21.673 | 64.049 | 1.00 51.00 | |
| | ATOM | 15585 | CE | LYS C | | 29.958 | 20.230 | 63.586 | 1.00 56.39 | |
| | MOTA | 15588 | NZ | LYS C | 224 | | 19.360 | 63.812 | | |
| | MOTA | 15592 | C, | LYS C | 224 | 27.355 | 24.489 | 61.644 | 1.00 50.04 | |
| 50 | ATOM | 15593 | 0 | LYS C | 224 | 27.279 | 23.799 | 60.619 | 1.00 44.69 | |
| | MOTA | 15594 | N | SER C | 225 | 27.960 | 25.684 | 61.708 | 1.00 50.25 | |
| • | ATOM | 15596 | CA | SER C | 225 | 28.747 | 26.210 | 60.604 | 1.00 47.90 | |
| | ATOM | 15598 | CB | SER C | 225 | 28.098 | 27.468 | 60.076 | 1.00 47.14 | |
| | ATOM | 15601 | 0G | SER C | 225 | 26.865 | 27.124 | 59.460 | 1.00 52.47 | |
| 55 | ATOM | 15603 | С | SER C | 225 | 30.179 | 26.415 | 61.102 | 1.00 44.94 | С |
| | ATOM | 15604 | 0 | SER C | 225 | 30.396 | 27.152 | 62.055 | 1.00 47.22 | 0 |
| | ATOM | 15605 | N | ILE C | 226 | 31.149 | 25.745 | 60.479 | 1.00 45.19 | |
| | MOTA | 15607 | CA | ILE C | 226 | 32.557 | 25.868 | 60.888 | 1.00 43.93 | |
| | ATOM | 15609 | CB | ILE (| 226 | 33.045 | 24.557 | 61.593 | 1.00 39.91 | |
| 60 | ATOM | 15611 | CG1 | ILE C | | 33.415 | 23.500 | 60.579 | 1.00 39.64 | |
| | ATOM | 15614 | | ILE (| | 34.031 | 22.226 | 61.231 | 1.00 37.78 | C |
| | | | | | | | | | | |

| 5 | ATOM | 15618 | CG2 | ILE C | 226 | 31.999 | 24.023 | 62.556 | | 42.23 | | | С |
|------|------|---------|-----------|---------|-------|------------------|------------------|------------------|------|----------------|---|----|--------|
| _ | ATOM | 15622 | С | ILE C | 226 | 33.472 | 26.181 | 59.710 | | 43.36 | | | С |
| | MOTA | 15623 | | ILE C | | 33.060 | 26.084 | 58.545 | | 42.72 | - | | 0 |
| | ATOM | 15624 | | VAL C | | 34.717 | 26.544 | 60.020 | | 45.45 | | | N |
| | ATOM | 15626 | CA | VAL C | 227 | 35.743 | 26.881 | 59.000 | 1.00 | | | | С |
| 10 | ATOM | 15628 | CB | VAL C | 227 | 36.309 | 28.367 | 59.169 | | 47.46 | | | С |
| | ATOM | 15630 | CG1 | VAL C | 227 | 37.483 | 28.629 | 58.234 | | 46.44 | | | С |
| | ATOM | 15634 | | VAL C | | 35.241 | 29,399 | 58.940 | | 48.83 | | | C |
| | MOTA | . 15638 | С | VAL · C | 227 | 36.907 | 25.894 | 59.111 | | 44.62 | | | С |
| | MOTA | 15639 | - | VAL C | | 37.588 | 25.862 | | | 41.47 | | | 0 |
| 15 | ATOM | 15640 | | ASP C | | 37.146 | 25.120 | 58.043 | | 45.60 | • | | . N |
| | MOTA | 15642 | | ASP C | | 38.103 | 24.013 | 58.065 | | 43.43 | | | С |
| | ATOM | 15644 | | ASP C | | 37.291 | 22.734 | 58.217 | | 44.61 | • | | C |
| | ATOM | 15647 | | ASP C | | 38.162 | 21.501 | 58.399 | | 49.06 | | | C |
| • | MOTA | 15648 | | ASP C | | 39.346 | 21.674 | 58.748 | | 51.29 | | | 0 |
| 20 | MOTA | 15649 | | ASP C | • | 37.754 | 20.325 | 58.225 | | 48.80 | | | 0 |
| | MOTA | 15650 | | ASP C | | 39.059 | 23.867 | 56.868 | | 42.97 | | | C |
| | MOTA | 15651 | 0 | ASP C | | 38.667 | 23.383 | 55.830 | | 51.06 | | | O N |
| | MOTA | 15652 | N | SER C | | 40.319 | 24.264 | 57.035 | | 42.95 | | | |
| | ATOM | 15654 | CA | SER C | | 41.355 | 24.153 | 55.999 | | 42.72 | | | C |
| 25 · | MOTA | 15656 | CB | SER C | | 42.649 | 24.816 | 56.493 | | 45.39 | | | C |
| | ATOM | 15659 | OG | SER C | | 43.168 | 24.142 | 57.661 | | 48.69 | | | 0 |
| | MOTA | 15661 | С | SER C | | 41.719 | 22.733 | 55.619 | | 43.75 | | | C |
| | MOTA | 15662 | 0 | SER C | | 42.444 | 22.509 | 54.667 | | 44.82 | | | |
| | MOTA | 15663 | N | GLY C | | 41.256 | 21.765 | 56.389 | | 47.33 | | | И |
| 30 | MOTA | 15665 | CA | GLY C | | 41.472 | 20.366 | 56.072 | | 45.82 | | | C C |
| | ATOM | 15668 | С | GLY C | | 40.324 | 19.725 | 55.294 | | 47.37 | | | 0 |
| | MOTA | 15669 | 0 | GLY C | | 40.365 | 18.517 | 55.074 | | 50.08 | | | |
| | MOTA | 15670 | N | THR C | | 39.329 | 20.528 | 54.875 | | 50.13 | | | N C |
| | ATOM | 15672 | CA | THR C | | 38.127 | 20.075 | 54.126 | | 44.81 | | | C |
| 35 | MOTA | 15674 | СВ | THR C | | 36.847 | 20.427 | 54.846 | | 41.41 42.47 | | | o |
| | ATOM | 15676 | | THR C | | 36.874 | 19.913 | 56.171 | | | | | ç |
| | ATOM | 15678 | | THR C | | 35.737 | 19.674 | 54.262 | | 45.87 46.97 | | | Ċ |
| | ATOM | 15682 | C | THR C | | 38.097 | 20.737 21.973 | 52.773 52.653 | | 41.58 | | ٠. | ő |
| 40 | ATOM | 15683 | 0 | THR C | | 38.225 37.903 | | 51.755 | | 47.97 | | | N |
| 40 | ATOM | 15684 | N | THR C | | 38.114 | 20.336 | 50.382 | | 48.47 | | | C |
| | MOTA | 15686 | CA | THR C | | 38.315 | | 49.509 | | 47.83 | | | č |
| | ATOM | 15688 | CB OC1 | THR C | | 39.514 | | 49.871 | | 46.26 | | | o |
| | ATOM | 15690 | | THR C | | 38.589 | | 48.087 | | 52.26 | | | Ċ |
| 15 | ATOM | 15692 | | | 232 | 36.991 | | 49.741 | | 49.88 | | | C |
| 45 | ATOM | 15696 | C | THR C | | 37.264 | | 48.965 | | 52.26 | | | Ō |
| | ATOM | 15697 | O N | ASN C | | 35.743 | | 50.054 | | 47.73 | | | N |
| • | ATOM | 15698 | CA | ASN C | | | 21.318 | | | 44.90 | | | C |
| | ATOM | 15700 | | | | 33.570 | | 49.063 | | 44.37 | | | Ç. |
| 50 | MOTA | 15702 | CB | ASN C | | 34.025 | | 48.006 | | 47.43 | | | Č |
| 50 | MOTA | 15705 | CG | | | 35.051 | | 47.345 | | 52.27 | | | o |
| | MOTA | 15706 | | ASN C | | 33.216 | | 47.871 | | 47.91 | | | N |
| | ATOM | 15707 | | ASN C | | | 22.287 | | | 49.52 | | | C |
| | ATOM | 15710 | C | ASN C | | 34.283 | | 51.451 | | 51.70 | | | ō |
| 55 | MOTA | 15711 | 0 | LEU C | | 32.787 | | 49.792 | | 49.50 | | | N |
| 55 | ATOM | 15712 | N | | | 31.851 | | 50.561 | | 50.43 | | | C |
| | ATOM | 15714 | | LEU C | | 31.168 | | | | 49.25 | | | Č |
| | MOTA | 15716 | CB | LEU C | | 30.577 | | 50.268 | | 46.33 | | | · c |
| | MOTA | 15719 | CG | LEU (| | 29.479 | | 49.377 | | 40.51 | | | c |
| 60 | ATOM | 15721 | | LEU (| | 30.090 | | 51.667 | | 46.97 | | | Č |
| UU | MOTA | 15725 | | LEU (| | 30.852 | | 50.965 | | 49.62 | | | Č |
| | MOTA | 15729 | C | TEO (| , 234 | 50.032 | . 22.333 | 50.505 | 4.00 | | | | _ |

| | | | • | | | | | | | | | _ |
|-----|------|-------|-----|-------------|--------|--------|--------|--------|-------|---|---|----|
| 5 | ATOM | 15730 | 0 | LEU C 234 | 30.407 | 21.816 | 50.116 | 1.00.4 | | | | 0 |
| . • | ATOM | 15731 | N | ARG C 235 | 30.491 | 22.520 | 52.239 | 1.00 | 18.90 | | | N |
| | ATOM | 15733 | CA | ARG C 235 | 29.625 | 21.424 | 52.677 | 1.00 4 | 14.81 | | | С |
| | ATOM | 15735 | CB | ARG C 235 | 30.348 | 20.503 | 53.656 | 1.00 | 13.27 | | | С |
| | | | | ARG C 235 | 31.341 | 19.584 | 53.002 | 1.00 | 13.89 | | | С |
| | MOTA | 15738 | CG | ARG C 235 | 30.842 | 18.160 | 52.801 | 1.00 ! | | | | С |
| 10 | ATOM | 15741 | CD | | | 17.255 | 53.837 | 1.00 | | | | N |
| | MOTA | 15744 | NE | ARG C 235 | 31.337 | | 53.811 | 1.00 | | | | С |
| | MOTA | 15746 | CZ | ARG C 235 | 31.221 | 15.938 | | 1.00 | | | | N |
| | ATOM | 15747 | | ARG C 235 | 31.708 | 15.258 | 54.800 | 1.00 | | | | N |
| | ATOM | 15750 | NH2 | ARG C 235 | 30.623 | 15.297 | 52.831 | | | | | C |
| 15 | MOTA | 15753 | С | ARG C 235 | 28.396 | 21.986 | 53.309 | 1.00 | | | | Ö |
| | MOTA | 15754 | 0 | ARG C 235 | 28,468 | 22.809 | 54.227 | 1.00 | | | | |
| | ATOM | 15755 | N | LEU C 236 | 27.250 | 21.535 | 52.823 | 1.00 | | | | И |
| | ATOM | 15757 | CA | LEU C 236 | 26.029 | 22.121 | 53.291 | 1.00 | | | | C |
| | ATOM | 15759 | CB | LEU C 236 | 25.356 | 23.023 | 52.230 | 1.00 | | | | С |
| 20 | ATOM | 15762 | CG | LEU C 236 | 26.128 | 24.202 | 51.585 | | 44.63 | | | С |
| 20 | MOTA | 15764 | | LEU C 236 | 26.000 | 24.076 | 50.073 | 1.00 | 44.76 | | | С |
| | ATOM | 15768 | | LEU C 236 | 25.626 | 25.572 | 52.036 | 1.00 | 45.65 | | | С |
| | | | C | LEU C 236 | 25.108 | 21.049 | 53.643 | 1.00 | 43.06 | | | Ç |
| | MOTA | 15772 | | LEU C 236 | 24.992 | 20.025 | 52.998 | 1.00 | | | | 0 |
| 25 | ATOM | 15773 | 0 | PRO C 237 | 24.421 | 21.296 | 54.709 | 1.00 | | | | N |
| 25 | MOTA | 15774 | N | | | 20.404 | 55.125 | 1.00 | | | | С |
| | MOTA | 15775 | CA | PRO C 237 | 23.369 | | 56.095 | 1.00 | | | • | C |
| | MOTA | 15777 | CB | PRO C 237 | 22.620 | 21.271 | | | 39.72 | | | ·Č |
| | MOTA | 15780 | CG | PRO C 237 | 23.724 | 22.119 | 56.697 | | 39.54 | | | č |
| | MOTA | 15783 | CD. | | 24.594 | 22.448 | 55.598 | | | | | c |
| 30 | ATOM | 15786 | С | PRO C 237 | 22.468 | 19.981 | 53.957 | | 56.07 | | | Ö |
| | ATOM | 15787 | 0 | PRO C 237 | 22.182 | 20.767 | 53.053 | | 61.19 | | | |
| | MOTA | 15788 | N | LYS C 238 | 22.049 | 18.724 | 54.011 | | 64.48 | | | N |
| | ATOM | 15790 | CA | LYS C 238 | 21.060 | 18.088 | 53.117 | | 67 74 | | | С |
| | MOTA | 15792 | CB | LYS C 238 | 20.344 | 16.981 | 53.939 | | 70.89 | | | c |
| 35 | MOTA | 15795 | CG | LYS C 238 | 19.364 | 16.043 | 53.183 | | 75.72 | | | С |
| 50 | MOTA | 15798 | CD | LYS C 238 | 20.022 | 15.198 | 52.057 | | 77.64 | | | С |
| | ATOM | 15801 | CE | LYS C 238 | 19.238 | 13.898 | 51.786 | 1.00 | 76.46 | | | С |
| | ATOM | 15804 | NZ | LYS C 238 | 19.681 | 13.117 | 50.588 | | 74.66 | | | N |
| | ATOM | 15808 | C | LYS C 238 | 20.005 | 19.015 | 52.472 | 1.00 | 67.39 | | | С |
| 40 | ATOM | 15809 | ŏ | LYS C 238 | 19.814 | 19.005 | 51.247 | 1.00 | 67.71 | | | 0 |
| 710 | | 15810 | N. | LYS C 239 | 19.303 | 19.801 | | 1.00 | 64.13 | | | N |
| | MOTA | 15812 | CA | LYS C 239 | 18.305 | 20.683 | 52.716 | | 64.27 | | | Ċ |
| | ATOM | | | LYS C 239 | 17.338 | 21.171 | 53.792 | | 68.69 | | | С |
| | ATOM | 15814 | CB | | 16.086 | 20.292 | 53.968 | | 74.28 | | | С |
| 45 | ATOM | 15817 | CG | LYS C 239 | 15.063 | 20.977 | 54.894 | | 76.92 | | | С |
| 45 | MOTA | 15820 | CD | LYS C 239 | 14.640 | 22.366 | 54.381 | | 76.03 | | | C |
| | ATOM | 15823 | CE | LYS C 239 | | 23.177 | 55.415 | | 74.75 | | | N |
| | ATOM | 15826 | NZ | LYS C 239 | 13.915 | | | | 62.66 | | • | C |
| | MOTA | 15830 | С | LYS C 239 | 18.918 | 21.886 | 52.013 | | | | | ő |
| | ATOM | 15831 | О | LYS C 239 | 18.495 | | 50.903 | | 62.29 | | | |
| 50 | MOTA | 15832 | N | VAL C 240 | 19.913 | 22.528 | | | 56.54 | | | N |
| | ATOM | 15834 | CA | VAL C 240 | 20.450 | | 52.039 | | 48.20 | | | C |
| | ATOM | 15836 | CB | VAL C 240 | 21.459 | | 52.876 | | 47.96 | | | C |
| | ATOM | 15838 | CG: | 1 VAL C 240 | 21.799 | | 52.198 | | 51.82 | | | C |
| | ATOM | | CG | 2 VAL C 240 | 20.934 | 24.744 | 54.268 | | 49.07 | | | С |
| 55 | MOTA | | | VAL C 240 | 21.110 | 23.315 | 50.780 | | 44.11 | | | C |
| | ATOM | | | VAL C 240 | 21.003 | | 49.756 | | 40.57 | • | | 0 |
| | ATOM | | | PHE C 241 | 21.797 | | 50.839 | 1.00 | 43.45 | | | N |
| | ATOM | | | PHE C 241 | 22.457 | | 49.645 | 1.00 | 44.85 | | | С |
| | ATOM | | | | 23.107 | | | 1.00 | 44.07 | | | С |
| 60 | ATOM | | | · · | 23.738 | | | • | 44.31 | | | С |
| UU | | | | 1 PHE C 241 | 25.015 | | | | 40.53 | | | С |
| | ATOM | 1000 | CD | - Lui C 241 | 20.020 | | | | | | | |

| | | . | | | | | | | | | | |
|-------------|--------|----------|-----|---------|-----|--------|--------|--------|------|-------|---|----|
| 5 | ATOM . | 15858 | CE1 | PHE C 2 | 241 | 25.575 | 19.460 | 47.272 | 1.00 | 42.85 | | С |
| _ | ATOM | 15860 | CZ | PHE C 2 | | 24.879 | 18.608 | 46.499 | 1.00 | 35.50 | | С |
| | MOTA | 15862 | CE2 | PHE C 2 | | 23.628 | 18.323 | 46.804 | 1.00 | 37.83 | | С |
| | ATOM | 15864 | CD2 | PHE C 2 | 241 | 23.039 | 18.897 | 47.899 | 1.00 | 44.17 | | С |
| | ATOM | 15866 | С | PHE C 2 | 241 | 21.495 | 21.587 | 48.488 | 1.00 | 46.73 | | С |
| 10 | ATOM | 15867 | | PHE C 2 | 241 | 21.880 | 21.762 | 47.328 | 1.00 | 46.03 | | Ó |
| 10 | ATOM | 15868 | N | GLU C 2 | | 20.241 | 21.294 | 48.824 | 1.00 | 50.74 | | N |
| | ATOM | 15870 | CA | GLU C 2 | | 19.228 | 20.899 | 47.851 | 1.00 | 51.33 | | С |
| | ATOM | 15872 | СВ | GLU C 2 | | 18.100 | 20.168 | 48.570 | 1.00 | 56.02 | | С |
| | ATOM | 15875 | CG | GLU C 2 | | 18.214 | 18.657 | 48.515 | 1.00 | 62.01 | | C |
| 15 | ATOM | 15878 | CD | GLU C 2 | | 18.576 | 18.183 | 47.122 | 1.00 | 66.03 | | С |
| | ATOM | 15879 | | GLU C 2 | | 18.159 | 18.881 | 46.155 | 1.00 | 67.53 | | 0 |
| | ATOM | 15880 | | GLU C 2 | | 19.277 | 17.134 | 46.997 | 1.00 | 60.97 | | 0 |
| | ATOM | 15881 | | GLU C 2 | | 18.645 | 22.076 | 47.116 | 1.00 | 50.90 | | С |
| • | ATOM | 15882 | Ō | GLU C 2 | | 18.470 | 22.057 | 45.901 | 1.00 | 46.64 | | 0 |
| 20 | ATOM | 15883 | N | ALA C 2 | | 18.337 | 23.100 | 47.883 | | 47.93 | | N |
| 20 | ATOM | 15885 | CA | ALA C 2 | | 17.831 | 24.310 | 47.324 | 1.00 | 50.32 | | С |
| | ATOM | 15887 | СВ | ALA C 2 | | 17.431 | 25.228 | 48.429 | 1.00 | 49.97 | | С |
| | ATOM | 15891 | C | ALA C 2 | | 18.932 | 24.932 | 46.484 | 1.00 | 53.72 | | С |
| | ATOM | 15892 | 0 | ALA C 2 | | 18.694 | 25.406 | 45.376 | 1.00 | 58.27 | | 0 |
| 25 | ATOM | 15893 | N | ALA C 2 | | 20.142 | 24.925 | 47.020 | 1.00 | 55.49 | | N |
| | ATOM | 15895 | CA | ALA C 2 | | 21.270 | 25.524 | 46.335 | 1.00 | 53.08 | | С |
| | ATOM | 15897 | СВ | ALA C 2 | | 22.505 | 25.573 | 47.229 | 1.00 | 55.11 | | Ç |
| | ATOM | 15901 | c | ALA C 2 | | 21.575 | 24.821 | 45.057 | 1.00 | 53.02 | | С |
| | ATOM | 15902 | ō | ALA C 2 | | 21.779 | 25.481 | 44.073 | 1.00 | 60.49 | | 0 |
| 30 | ATOM | 15903 | N | VAL C 2 | | 21.608 | 23.495 | 45.025 | 1.00 | 56.92 | | N |
| | ATOM | 15905 | CA | VAL C 2 | | 21.907 | 22.825 | 43.748 | 1.00 | 53.60 | | C |
| | ATOM | 15907 | СВ | VAL C 2 | | 22.025 | 21.300 | 43.842 | 1.00 | 55.63 | | С |
| | ATOM | 15909 | | VAL C 2 | | 22.667 | 20.709 | 42.554 | 1.00 | 54.38 | | С |
| | ATOM | 15913 | | VAL C 2 | | 22.819 | 20.900 | 45.014 | 1.00 | 58.96 | | С |
| 35 | ATOM | 15917 | C | VAL C 2 | | 20.804 | 23.069 | 42.734 | 1.00 | 55.12 | | C |
| - | ATOM | 15918 | 0 | VAL C 2 | 245 | 21.060 | 22.974 | 41.544 | 1.00 | 58.24 | • | 0 |
| | ATOM | 15919 | N | LYS C 2 | | 19.574 | 23.356 | 43.160 | 1.00 | 52.47 | | N |
| | ATOM | 15921 | CA | LYS C 2 | | 18.549 | 23.620 | 42.157 | 1.00 | 58.91 | | С |
| | ATOM | 15923 | СВ | LYS C 2 | 246 | 17.129 | 23.817 | 42.754 | 1.00 | 62.86 | | C |
| 40 | ATOM | 15926 | CG | LYS C 2 | 246 | 16.324 | 22.600 | 43.183 | 1.00 | 70.41 | | С |
| | ATOM | 15929 | CD | LYS C 2 | 246 | 16.388 | 21.363 | 42.223 | 1.00 | 76.82 | | С |
| | ATOM | 15932 | CE | LYS C 2 | 246 | 17.595 | 20.433 | 42.499 | 1.00 | 77.01 | | С |
| | ATOM | 15935 | NZ | LYS C 2 | 246 | 17.683 | 19.311 | 41.510 | | 75.94 | | N |
| • | ATOM | 15939 | C | LYS C 2 | 246 | 18.944 | 24.940 | 41.486 | | 56.47 | | С |
| 45 | MOTA | 15940 | 0 | LYS C 2 | 246 | 19.066 | 25.062 | 40.257 | | 59.03 | | 0 |
| | ATOM | 15941 | N | SER C | 247 | 19.153 | 25.920 | 42.348 | • | 47.24 | | N |
| | ATOM | 15943 | CA | SER C | | 19.348 | 27.272 | 41.934 | | 47.24 | | C. |
| | MOTA | 15945 | CB | SER C | 247 | 19.509 | 28.132 | 43.169 | | 47.72 | | С |
| | ATOM | 15948 | OG | SER C | 247 | 19.430 | 29.494 | 42.810 | | 53.48 | | 0 |
| 50 | ATOM | 15950 | С | SER C | 247 | 20.563 | 27.421 | 41.042 | | 47.61 | | С |
| | MOTA | 15951 | 0 | SER C | 247 | 20.552 | 28.143 | 40.030 | | 48.26 | | 0 |
| | ATOM | 15952 | N | ILE C | 248 | 21.612 | 26.730 | 41.432 | | 40.55 | | N |
| | MOTA | 15954 | CA | ILE C. | 248 | 22.802 | 26.795 | 40.710 | 1.00 | 39.34 | | С |
| | ATOM | 15956 | CB | ILE C | 248 | 23.804 | 25.942 | 41.355 | 1.00 | 39.28 | | С |
| 55 | ATOM | 15958 | CG1 | ILE C | 248 | 24.164 | 26.530 | 42.675 | 1.00 | 37.69 | | С |
| | MOTA | 15961 | CD1 | ILE C | 248 | 25.595 | 26.384 | 42.926 | 1.00 | 40.41 | | С |
| _ | MOTA | 15965 | CG2 | ILE C | | 25.073 | 25.940 | 40.565 | | 45.18 | | С |
| | ATOM | 15969 | С | ILE C | 248 | 22.498 | 26.311 | 39.348 | | 47.60 | | С |
| | MOTA | 15970 | 0 | ILE C | 248 | 22.793 | 27.013 | 38.398 | | 52.36 | | О |
| 60 . | MOTA | 15971 | N | LYS C | 249 | 21.894 | 25.118 | 39.244 | | 54.81 | | N |
| | ATOM | 15973 | CA | LYS C | 249 | 21.619 | 24.488 | 37.939 | 1.00 | 52.55 | | С |
| | | | | | | | | | | | | |

| | | * | | | | | | | - 00 | 04 | | | С | |
|----|-------------|---------|-----|-------|-------|--------|---------|---------|--------------|----------------|---|-----|-----|-----|
| 5 | ATOM | 15975 | CB | LYS C | 249 | 20.735 | 23.263 | | 1.00 | | | | C | • |
| , | | | CG | LYS C | 249 | 21.397 | 21.980 | | 1.00 | 60.13 62.40 | | | Č | |
| | | | CD | LYS С | 249 | 20.426 | 20.783 | | 1.00 1.00 | | | | č | |
| | | 15984 | CE | LYS C | 249 | 20.792 | 19.557 | 39.172 | | | | | N | |
| | | 15987 | | LYS C | | 19.732 | 19.211 | 40.190 | | 73.03 | | | c | |
| 10 | • • • • • • | 15991 | С | LYS C | | 20.837 | 25.463 | 37.110 | | 51.86 | | | ő | |
| 10 | | 15992 | 0 | LYS C | 249 | 21.209 | 25.796 | 35.990 | | 56.70 | | | N | |
| | ATOM | 15993 | N | ALA C | 250 | 19.737 | 25.924 | 37.683 | | 44.72 | | | C | |
| | ATOM | 15995 | CA | ALA C | 250 | 18.871 | 26.855 | 36.999 | 1.00 | 43.29 | | • | C | |
| | ATOM | 15997 | CB | ALA C | | 17.850 | 27.442 | 37.977 | 1.00 | 38.29 | | | C | |
| 15 | | 16001 | C | ALA C | | 19.696 | 27.950 | 36.371 | 1.00 | 45.27 | | | . 0 | |
| 15 | MOTA | 16002 | ŏ | ALA C | | 19.535 | 28.253 | 35.199 | | 46.37 | | | N | |
| | MOTA | 16002 | N | ALA C | | 20.600 | 28.539 | 37.153 | 1.00 | 44.64 | | , | | |
| | ATOM | | CA | ALA C | | 21.362 | 29.667 | 36.658 | 1.00 | 42.02 | | | C | |
| | MOTA | 16005 | CB | ALA C | | 22.173 | 30.242 | 37.739 | 1.00 | 39.56 | | | · C | |
| | MOTA | 16007 | CD | ALA C | | 22.237 | 29.272 | 35.492 | | 44.55 | | | C | |
| 20 | MOTA | 16011 | o | ALA C | | 22.459 | 30.029 | 34.574 | | 53.96 | | | 0 | |
| | ATOM | 16012 | | SER C | | 22.716 | 28.059 | 35.523 | 1.00 | 48.25 | | | .N | |
| | ATOM | 16013 | N | SER C | 252 | 23.581 | 27.567 | 34.487 | | 50.72 | | | C | |
| | ATOM | 16015 | CA | SER (| | 24.561 | 26.537 | 35.095 | 1.00 | 50.46 | | . , | C | |
| | MOTA | 16017 | CB | SER C | | 24.087 | 26.053 | 36.372 | 1.00 | 50.66 | | | | |
| 25 | MOTA | 16020 | OG | | 252 | 22.746 | 26.890 | 33.427 | 1.00 | 51.45 | | | | ; |
| | MOTA | 16022 | C | | 252 | 23.305 | 26.186 | 32.595 | | 54.49 | | | C | |
| | MOTA | 16023 | 0 | SER C | 202 | 21.428 | 27.104 | 33.448 | 1.00 | 52.44 | | | 1 | |
| | MOTA | 16024 | N | | C 253 | 20.502 | 26.337 | 32.588 | 1.00 | 55.69 | | | (| |
| | MOTA | 16026 | CA | SER | C 253 | 19.025 | 26.589 | 32.995 | 1.00 | 58.26 | | | (| |
| 30 | MOTA | 16028 | CB | SER | C 253 | 18.469 | 27.826 | 32.540 | | 55.32 | | | |) |
| | MOTA | 16031 | QG | SER | C 253 | 20.673 | 26.458 | 31.073 | | 58.55 | | | (| C |
| | MOTA | 16033 | С | | C 253 | 19.693 | 26.428 | 30.343 | | 67.47 | | | (| 0 |
| | MOTA | 16034 | 0 | | C 253 | 21.917 | 26.600 | | | 62.21 | | | | N |
| | MOTA | 16035 | N | | C 254 | 22.258 | 26.667 | 29.181 | | 64.73 | | | | С |
| 35 | MOTA | 16037 | CA | THR | C 254 | 22.230 | 27.939 | 28.896 | | 66.84 | | | 1 | С |
| | MOTA | 16039 | CB | | C 254 | 24.215 | | | | 71.03 | | | | 0 |
| | MOTA | 16041 | | 1 THR | C 254 | 22.183 | | | 1.00 | 72.72 | | | | C , |
| | MOTA | 16043 | CG: | 2 THR | C 254 | 23.294 | | | 1.00 | 68.84 | | | | С |
| - | MOTA | 16047 | С | | C 254 | 23.746 | | | 1.00 | 68.20 | | | | 0 |
| 40 | MOTA | 16048 | 0 | | C 254 | 23.740 | | | | 69.98 | | | | N |
| | MOTA | 16049 | N | | C 255 | 24.513 | | | | 69.15 | | | | C, |
| | ATOM | | CA | GLU | C 255 | 25.990 | | | | 69.01 | | | | C |
| | MOTA | | | | C 255 | 26.765 | | | | 73.89 | | | | C |
| | MOTA | | | | C 255 | 28.135 | | | | 0 80.19 | | | | C |
| 45 | ATOM | 16059 | | GLU | C 255 | 28.259 | | | | 0 77.88 | | | - | 0 |
| • | ATOM | 16060 | | 1 GLU | C 255 | 29.078 | | | • | 0 75.03 | | | | Ö, |
| | ATOM | | OE | 2 GLU | C 255 | | | | | 0 68.56 | | | | C |
| | ATOM | 16062 | | GĻŪ | C 255 | 23.813 | | | | 0 63.70 | | | | 0 |
| • | ATOM | | 0 | GLU | C 255 | 23.260 | | | 1.0 | 0 69.73 | | | | N |
| 50 | ATOM | 16064 | N | LYS | C 256 | 23.79 | | | 1 0 | 0 69.57 | | | | С |
| | ATOM | 1 16066 | CP | LYS | C 256 | 23.14 | | | 1.0 | 0 71.79 | | | | C |
| - | ATOM | 1 16068 | CE | LYS | C 256 | 21.87 | | | 1 1 0 | 0 73.04 | | | : | C |
| | ATOM | | CC | LYS | C 256 | 20.81 | | | _ | 0 75.70 | - | | | C |
| | ATOM | | |) LYS | C 256 | 20.47 | | | _ | 0 74.59 | | | | C |
| 55 | | | | | C 256 | 19.06 | | | - | 10 14.73 | | | | N |
| | ATON | | | LYS | C 256 | 18.58 | | | | 0 76.39 | | | | C |
| | ATO | | | LYS | C 256 | 24.21 | | | _ | 0 67.18 | | | | o |
| | ATO | | | LYS | C 256 | 25.20 | | | | 0 58.20 | | | | N |
| | ATO | | | PHE | C 257 | 24.07 | | | | 0 68.64 | | | | C |
| 60 | | | | A PHE | C 257 | 25.04 | | | | 0 69.01 | | | | Ċ |
| | ATO | | | в РНЕ | C 257 | 26.00 | 5 19.05 | 0 34.00 | 9 1.6 | 00 72.10 | | | | ~ |
| | | | | | | | | | | | | | | |

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| 5 | ATOM | 16093 | CG | PHE C 257 | 26.744 | 20.209 | 33.362 | 1.00 69.14 | | С |
|-----|------|-------|-----|-------------|------------------|------------------|--------|--------------------------|---|-----|
| ٠. | ATOM | 16094 | | PHE C 257 | 26.419 | 21.522 | 33.680 | 1.00 69.09 | | С |
| | ATOM | 16096 | | PHE C 257 | 27.086 | 22.590 | 33.094 | 1.00 67.65 | | С |
| | ATOM | 16098 | | PHE C 257 | 28.091 | 22.354 | 32.180 | 1.00 71.28 | | С |
| | ATOM | 16100 | | PHE C 257 | 28.431 | 21.043 | 31.849 | 1.00 72.57 | | С |
| 10 | ATOM | 16102 | | PHE C 257 | 27.755 | 19.980 | 32.439 | 1.00 71.04 | | С |
| 10 | ATOM | 16104 | C | PHE C 257 | 24.335 | 17.131 | 33.647 | 1.00 69.41 | | С |
| | ATOM | 16105 | ō | PHE C 257 | 23.173 | 17.187 | 34.100 | 1.00 68.36 | | 0 |
| | ATOM | 16106 | N | PRO C 258 | 25.041 | 16.022 | 33.594 | 1.00 68.72 | | N |
| | ATOM | 16107 | CA | PRO C 258 | 24.559 | 14.751 | 34.139 | 1.00 72.08 | | C |
| 15 | ATOM | 16109 | СВ | PRO C 258 | 25.649 | 13.798 | 33704 | 1.00 72.60 | | С |
| 13 | MOTA | 16112 | CG | PRO C 258 | 26.863 | 14.705 | 33.627 | 1.00 72.00 | | С |
| | MOTA | 16115 | CD | PRO C 258 | 26.363 | 15.901 | 32.963 | 1.00 68.28 | | С |
| | ATOM | 16118 | C | PRO C 258 | 24.507 | 14.757 | 35.662 | 1.00 74.57 | | С |
| | | 16119 | Ö | PRO C 258 | 25.438 | 15.317 | 36.245 | 1.00 75.66 | | 0 |
| 20 | ATOM | 16120 | N | ASP C 259 | 23.479 | 14.151 | 36.272 | 1.00 75.85 | | N. |
| 20 | ATOM | | CA | ASP C 259 | 23.355 | 14.015 | 37.747 | 1.00 77.50 | • | C |
| | MOTA | 16122 | CB. | ASP C 259 | 22.436 | 12.845 | 38.118 | 1.00 77.91 | | С |
| • • | MOTA | 16124 | | ASP C 259 | 20.964 | 13.134 | 37.904 | 1.00 80.16 | | С |
| | MOTA | 16127 | CG | ASP C 259 | 20.559 | 14.322 | 37.914 | 1.00 84.49 | | . 0 |
| 25 | MOTA | 16128 | | ASP C 259 | 20.333 | 12.206 | 37.727 | 1.00 74.07 | | Ō |
| 25 | MOTA | 16129 | | ASP C 259 | 24.649 | 13.750 | 38.543 | 1.00 77.00 | | C |
| | ATOM | 16130 | С | | 24.727 | 14.079 | 39.732 | 1.00 79.56 | | ō |
| | ATOM | 16131 | 0 | ASP C 259 | 25.648 | 13.148 | 37.914 | 1.00 75.01 | | N |
| | MOTA | 16132 | N | GLY C 260 | 26.852 | 12.769 | 38.636 | 1.00 75.71 | | c |
| 20 | ATOM | 16134 | CA | GLY C 260 | 27.782 | 13.929 | 38.922 | 1.00 74.37 | | Č |
| 30 | ATOM | 16137 | C | GLY C 260 | 28.535 | 13.929 | 39.919 | 1.00 75.33 | | ŏ |
| | MOTA | 16138 | 0 | GLY C 260 | | 14.918 | 38.035 | 1.00 69.34 | | N |
| | ATOM | 16139 | N | PHE C 261 | 27.730 | | 38.171 | 1.00 62.53 | | c |
| | ATOM | 16141 | CA | PHE C 261 | 28.550 | 16.095 | 36.990 | 1.00 63.25 | | Ċ |
| ~ ~ | ATOM | 16143 | CB | PHE C 261 | 28.341 | 17.037 18.334 | 37.098 | 1.00 63.23 | | , č |
| 35 | ATOM | 16146 | CG | PHE C 261 | 29.079 | 18.360 | 37.184 | 1.00 57.93 | | č |
| | ATOM | 16147 | | PHE C 261 | 30.455 | 19.557 | 37.104 | 1.00 55.60 | • | · C |
| | ATOM | 16149 | | PHE C 261 | 31.129 30.424 | 20.732 | 37.293 | 1.00 55.30 | | č |
| | ATOM | 16151 | CZ | PHE C 261 | | 20.732 | 37.210 | 1.00 56.24 | | Č |
| 40 | ATOM | 16153 | | PHE C 261 | 29.056 28.393 | 19.522 | 37.110 | 1.00 55.44 | | č |
| 40 | ATOM | 16155 | | PHE C 261 | | 16.693 | 39.413 | 1.00 58.82 | | č |
| | ATOM | 16157 | C | PHE C 261 | 28.026 | 16.758 | 40.395 | 1.00 50.02 | | Ö |
| | ATOM | 16158 | 0 . | PHE C 261 | 28.717 | 17.095 | 39.384 | 1.00 58.00 | | N |
| | ATOM | 16159 | N | TRP C 262 | 26.772 | 17.725 | 40.536 | 1.00 59.65 | | C |
| 40 | MOTA | 16161 | CA | TRP C 262 | .26.179 | 18.071 | 40.336 | 1.00 59.05 | | č |
| 45 | ATOM | 16163 | CB | TRP C 262 | 24.722 | 19.084 | 39.179 | 1.00 67.86 | | Č |
| | ATOM | 16166 | | TRP C 262 | 24.498 | | 38.046 | 1.00 69.53 | | Č |
| | ATOM | 16167 | | TRP C 262 | 23.762 | 18.900 20.038 | 37.278 | 1.00 70.01 | | N |
| | ATOM | 16169 | NE1 | | 23.775 | 77 7 | | | | C |
| | ATOM | 16171 | | TRP C 262 | 24.527 | 20.992 | 37.910 | 1.00 68.68 1.00 67.00 | | c |
| 50 | ATOM | 16172 | | TRP C 262 | 24.995 | 20.427 | 39.113 | | | c |
| | MOTA | 16173 | | TRP C 262 | 25.793 | 21.210 | 39.941 | 1.00 69.48 | | c |
| | ATOM | 16175 | | TRP C 262 | 26.091 | 22.516 | 39.547 | 1.00 69.43 | | c |
| | ATOM | 16177 | | TRP C 262 | 25.608 | 23.038 | 38.351 | 1.00 66.24 | | c |
| | MOTA | 16179 | | TRP C 262 | 24.830 | 22.295 | 37.520 | 1.00 66.76 | | |
| 55 | ATOM | 16181 | C | TRP C 262 | 26.284 | 16.847 | 41.766 | 1.00 58.97 | | C |
| | MOTA | 16182 | 0 | TRP C 262 | 26.059 | 17.301 | 42.869 | 1.00 57.31 | | 0 |
| | ATOM | 16183 | N | LEU C 263 | 26.601 | 15.574 | 41.597 | 1.00 65.06 | | N |
| | ATOM | 16185 | CA | LEU C 263 | 26.806 | 14.727 | 42.767 | 1.00 67.45 | | C |
| | ATOM | 16187 | СВ | LEU C 263 | 26.279 | 13.332 | 42.533 | 1.00 68.47 | | C |
| 60 | ATOM | 16190 | CG | LEU C 263 | 24.933 | | 43.225 | 1.00 72.82 | | C |
| | ATOM | 16192 | CD1 | . LEU C 263 | 24.425 | 11.685 | 42.977 | 1.00 71.73 | , | · C |

| 5 | MOTA | 16196 | CD2 | LEU (| C 263 | | 25.028 | 13.405 | 44.740 | 1.00 73.38 | C |
|----|-------------------|-------|-----|-------|-------|---|--------|--------|--------|------------|--------|
| | ATOM | 16200 | С | LEU (| C 263 | | 28.268 | 14.668 | 43.160 | 1.00 70.29 | С |
| | MOTA | 16201 | 0 | | C 263 | | 28.647 | 13.948 | 44.076 | 1.00 72.79 | 0 |
| | ATOM | 16202 | N | GLY · | C 264 | | 29.083 | 15.429 | 42.449 | 1.00 70.41 | N |
| | ATOM | 16204 | CA | | C 264 | • | 30.488 | 15.522 | 42.741 | 1.00 72.58 | С |
| 10 | MOTA | 16207 | С | | C 264 | | 31.254 | 14.276 | 42.369 | 1.00 74.99 | С |
| 10 | ATOM | 16208 | ō | | C 264 | | 32.427 | 14.136 | 42.728 | 1.00 77.68 | . 0 |
| | ATOM | 16209 | N | | C 265 | | 30.623 | 13.377 | 41.627 | 1.00 76.35 | N |
| | ATOM | 16211 | CA | | C 265 | | 31.266 | 12.097 | 41.328 | 1.00 75.36 | С |
| | ATOM | 16213 | СВ | | C 265 | • | 30.247 | 10.967 | 41.441 | 1.00 75.63 | С |
| 15 | ATOM | 16216 | CG | | C 265 | | 30.068 | 10.546 | 42.883 | 1.00 80.22 | C |
| 13 | | 16219 | CD | | C 265 | | 28.981 | 9.514 | 43.067 | 1.00 86.58 | Ċ |
| | ATOM | | | | C 265 | | 28.455 | 9.405 | 44.208 | 1.00 91.85 | . 0 |
| | ATOM | 16220 | | | C 265 | | 28.654 | 8.812 | 42.080 | 1.00 88.76 | · , 0 |
| | MOTA | 16221 | | | | | | 12.017 | 39.999 | 1.00 73.02 | Č |
| 20 | ATOM | 16222 | C | | C 265 | | 31.978 | 11.222 | 39.835 | 1.00 76.03 | ŏ |
| 20 | MOTA | 16223 | 0 | | C 265 | | 32.902 | | 39.048 | 1.00 72.24 | . и |
| | ATOM | 16224 | N | | C 266 | | 31.566 | 12.831 | | 1.00 72.24 | · c |
| | MOTA | 16226 | CA | | C 266 | | 32.162 | 12.771 | 37.730 | 1.00 75.94 | Č |
| ٠. | MOTA | 16228 | CB | | C 266 | | 31.280 | 12.063 | 36.723 | | C |
| | MOTA | 16231 | CG | | C 266 | | 29.788 | 12.214 | 36.972 | 1.00 81.31 | c |
| 25 | MOTA | 16234 | CD | | C 266 | | 29.003 | 11.021 | 36.409 | 1.00 87.99 | |
| | ATOM | 16235 | | | C 266 | | 28.246 | 10.351 | 37.140 | 1.00 89.26 | . 0 |
| | MOTA | 16236 | | | C 266 | | 29.191 | 10.748 | 35.112 | 1.00 87.50 | N |
| • | MOTA | 16239 | С | | C 266 | | 32.393 | 14.164 | 37.330 | 1.00 69.61 | |
| | MOTA | 16240 | 0 | | C 266 | | 31.739 | 15.075 | 37.808 | 1.00 71.73 | 0 |
| 30 | MOTA | 16241 | N | | C 267 | | 33.331 | 14.334 | 36.433 | 1.00 68.39 | N |
| | MOTA | 16243 | CA | | C 267 | | 33.829 | 15.649 | 36.183 | 1.00 65.70 | . C |
| | MOTA | 16245 | CB | | C 267 | | 35.351 | 15.611 | 36.200 | 1.00 66.35 | C |
| | MOTA | 16248 | CG | | C 267 | | 35.956 | 14.641 | 35.211 | 1.00 65.47 | C |
| | ATOM | 16250 | | | C 267 | | 35.336 | 14.904 | 33.871 | 1.00 70.86 | C |
| 35 | MOTA | 16254 | CD2 | | C 267 | | 37.458 | 14.823 | 35.131 | 1.00 67.21 | C |
| | ATOM | 16258 | С | | C 267 | | 33.306 | 16.140 | 34.883 | 1.00 66.62 | c |
| | ATOM | 16259 | 0 | | C 267 | | 32.568 | 15.458 | 34.196 | 1.00 68.94 | 0 |
| | MOTA | 16260 | N | VAL | C 268 | | 33.695 | 17.344 | 34.540 | 1.00 68.75 | N |
| | ATOM | 16262 | CA | | C 268 | | 33.215 | 17.954 | 33.335 | 1.00 69.12 | Ċ |
| 40 | MOTA | 16264 | CB | VAL | C 268 | | 32.183 | 19.052 | 33.644 | 1.00 65.32 | . С |
| | MOTA | 16266 | CG1 | VAL | C 268 | | 31.593 | 19.635 | 32.397 | 1.00 67.75 | · , C |
| | MOTA | 16270 | CG2 | VAL | C 268 | | 31.078 | 18.451 | 34.429 | 1.00 67.90 | C |
| | MOTA | 16274 | С | VAL | C 268 | | 34.486 | 18.491 | 32.781 | 1.00 70.89 | С |
| • | ATOM | 16275 | 0 | VAL | C 268 | | 35.439 | 18.735 | 33.524 | 1.00 77.01 | 0 |
| 45 | ATOM | 16276 | N | CYS | C 269 | | 34.523 | 18.651 | 31.477 | 1.00 70.74 | N |
| | AT _O M | 16278 | CA | | C 269 | | 35.718 | 19.116 | 30.843 | 1.00 71.32 | С |
| | ATOM | 16280 | CB | CYS | C 269 | | 36.480 | 17.899 | 30.275 | 1.00 71.55 | С |
| | ATOM | 16283 | SG | CYS | C 269 | | 37.148 | 16.791 | 31.565 | 1.00 73.61 | S |
| | ATOM | 16284 | С | CYS | C 269 | • | 35.301 | 20.102 | 29.776 | 1.00 69.44 | С |
| 50 | ATOM | 16285 | 0 | CYS | C 269 | | 34.176 | 20.064 | 29.278 | 1.00 72.40 | 0. |
| | ATOM | 16286 | N | | C 270 | | 36.213 | 20.994 | 29.444 | 1.00 68.17 | N |
| • | ATOM | 16288 | CA | TRP | C 270 | | 35.995 | 21.964 | 28.382 | 1.00 68.38 | . С |
| | ATOM | 16290 | СВ | | C 270 | | 35.565 | 23.322 | 28.933 | 1.00 68.67 | С |
| • | ATOM | 16293 | CG | | C 270 | | | 23.496 | 29.291 | 1.00 62.51 | C |
| 55 | MOTA | 16294 | | | C 270 | | 33.089 | 23.710 | 28.443 | 1.00 63.68 | C. |
| JJ | ATOM | 16296 | | | C 270 | | 31.925 | 23.859 | 29.159 | 1.00 67.43 | N |
| | ATOM | 16298 | | | C 270 | | 32.215 | 23.737 | 30.491 | 1.00 63.27 | c C |
| | ATOM | 16299 | | | C 270 | | 33.602 | 23.513 | 30.605 | 1.00 55.28 | č |
| | | 16300 | | | C 270 | | 34.151 | 23.368 | 31.866 | 1.00 54.22 | č |
| 60 | ATOM | 16300 | | | C 270 | | 33.332 | 23.436 | 32.950 | 1.00 54.22 | |
| 00 | ATOM | 16302 | | | C 270 | | 31.957 | 23.450 | 32.813 | 1.00 66.25 | |
| | MOTA | 10304 | ÇΠΖ | TWE | ~ 210 | | 31.331 | 23.033 | J2.0±J | 1.00,00.23 | v |

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| | | ×. | | | | | | | | | | | _ |
|-----|------|-------|-----|-------------|---|--------|--------|--------|------|-------|---|-----|----|
| 5 | ATOM | 16306 | CZ2 | TRP C 270 | | 31.382 | 23.807 | 31.588 | 1.00 | 62.56 | | | С |
| , | ATOM | 16308 | C | TRP C 270 | | 37.315 | 22.194 | 27.677 | 1.00 | 69.11 | | | С |
| | ATOM | 16309 | Ö | TRP C 270 | | 38.364 | 22.221 | 28.317 | 1.00 | 70.17 | | | 0 |
| | | | | GLN C 271 | | 37.267 | 22.369 | 26.360 | 1.00 | 71.22 | | | N |
| | ATOM | 16310 | N | | | 38.477 | 22.588 | 25.577 | | 69.66 | | | С |
| | ATOM | 16312 | CA | GLN C 271 | | 38.160 | 22.947 | 24.102 | | 73.03 | | | С |
| 10 | MOTA | 16314 | CB | GLN C 271 | | | | 23.172 | | 74.99 | | | Ç |
| | ATOM | 16317 | CG | GLN C 271 | | 37.704 | 21.781 | | | 83.57 | | | č |
| | ATOM | 16320 | CD | GLN C 271 | | 36.937 | 22.285 | 21.925 | | | | | 0 |
| | ATOM | 16321 | | GLN C 271 | | 37.039 | 23.476 | 21.547 | | 84.53 | | | |
| | ATOM | 16322 | NE2 | GLN C 271 | | 36.168 | 21.387 | 21.294 | | 80.42 | | | N |
| 15 | ATOM | 16325 | C | GLN C 271 | | 39.156 | 23.760 | 26.217 | | 68.22 | | | C. |
| | ATOM | 16326 | 0 | GLN C 271 | | 38.520 | 24.774 | 26.484 | | 67.07 | • | | Ò |
| | ATOM | 16327 | N | ALA C 272 | | 40.440 | 23.630 | 26.477 | | 71.24 | | | N |
| | ATOM | 16329 | CA | ALA C 272 | | 41.238 | 24.745 | 26.979 | 1.00 | 74.33 | | • . | C |
| ٠. | ATOM | 16331 | CB | ALA C 272 | | 42.541 | 24.817 | 26.195 | 1.00 | 74.83 | • | | C |
| 20 | | 16335 | C | ALA C 272 | | 40.536 | 26.126 | 26.949 | 1.00 | 74.62 | | | С. |
| 20 | ATOM | | | ALA C 272 | | 39.503 | | 26.311 | 1.00 | 71.88 | | | 0 |
| - | ATOM | 16336 | 0 | | | 41.122 | 27.065 | 27.674 | | 76.58 | | | N |
| | MOTA | 16337 | N | GLY C 273 | | | 28.420 | 27.784 | | 76.43 | | | С |
| | ATOM | 16339 | CA | GLY C 273 | | 40.622 | | | | 77.74 | | | Ċ |
| | MOTA | 16342 | С | GLY C 273 | | 39.135 | 28.692 | 27.603 | | 77.19 | | | Ö |
| 25 | MOTA | 16343 | Ó | GLY C 273 | | 38.736 | 29.848 | 27.710 | | | | | N |
| | ATOM | 16344 | N | THR C 274 | | 38.308 | 27.683 | 27.339 | | 76.54 | | | |
| | ATOM | 16346 | CA | THR C 274 | | 36.906 | 27.955 | 27.012 | | 76.18 | | | С |
| | ATOM | 16348 | CB | THR C 274 | | 36.486 | 27.048 | 25.827 | | 76.87 | | | С |
| | MOTA | 16350 | OG1 | THR C 274 | | 36.826 | 25.697 | 26.109 | | 74.47 | | | 0 |
| 30 | ATOM | 16352 | CG2 | THR C. 274 | | 37.342 | 27.319 | 24.594 | | 80.60 | | | С |
| - | ATOM | 16356 | С | THR C 274 | | 35.850 | 27.855 | 28.124 | 1.00 | 74.88 | | | С |
| | MOTA | 16357 | 0 | THR C 274 | | 34.676 | 28.013 | 27.834 | 1.00 | 80.88 | | | 0 |
| | ATOM | 16358 | Ŋ. | THR C 275 | | 36.229 | 27.608 | 29.375 | 1.00 | 70.60 | | | N |
| | | 16360 | CA | THR C 275 | | 35.217 | 27.451 | 30.431 | 1.00 | 64.63 | | | С |
| 35 | ATOM | 16362 | CB | THR C 275 | | 35.871 | 27.307 | 31.815 | 1.00 | 62.69 | | • | С |
| 33 | ATOM | | | THR C 275 | | 36.891 | 26.304 | 31.783 | | 58.88 | | | .0 |
| | ATOM | 16364 | | | | 34.862 | 26.769 | 32.815 | | 60.08 | | | С |
| | MOTA | 16366 | | THR C 275 | | 34.276 | 28.641 | 30.467 | | 59.66 | | | C |
| | MOTA | 16370 | C | THR C 275 | | | 29.751 | 30.547 | | 55.72 | | | o |
| 40 | ATOM | 16371 | 0 | THR C 275 | | 34.748 | 28.443 | 30.415 | | 56.44 | | | N |
| 40 | MOTA | 16372 | N | PRO C 276 | | 32.960 | | | | 55.38 | | | c |
| | MOTA | 16373 | CA | PRO C 276 | | 32.060 | 29.588 | 30.442 | | 57.23 | | | c |
| | MOTA | 16375 | CB | PRO C 276 | | 30.771 | 28.992 | 29.922 | | | | | c |
| | MOTA | 16378 | CG | PRO C 276 | | 30.763 | 27.713 | 30.617 | | 56.39 | | | |
| | ATOM | 16381 | CD | PRO C 276 | | 32.182 | 27.190 | 30.320 | | 57.95 | | | С |
| 45 | ATOM | 16384 | С | PRO C 276 | | 31.872 | 30.073 | 31.857 | | 52.50 | | | С |
| | ATOM | 16385 | 0 | PRO C 276 | | 30.764 | 30.068 | 32.414 | • | 56.88 | | | 0 |
| | ATOM | 16386 | N | TRP C 277 | | 32.951 | 30.527 | 32.459 | 1.00 | 49.70 | | | N |
| | ATOM | 16388 | CA | TRP C 277 | | 32.835 | 30.898 | 33.842 | 1.00 | 48.70 | | | С |
| | ATOM | 16390 | СВ | TRP C 277 | | 34.047 | 31.691 | 34.288 | 1.00 | 48.72 | | | С |
| 50 | ATOM | 16393 | | TRP C 277 | | 35.377 | 30.992 | 34.300 | 1.00 | 42.99 | | | С |
| 50 | ATOM | 16394 | | TRP C 277 | • | 36.452 | 31.282 | 33.497 | 1.00 | 44.54 | | | С |
| | | | | TRP C 277 | | 37.517 | 30.463 | 33.795 | | 40.79 | | | N |
| | ATOM | 16396 | | | | 37.153 | 29.623 | 34.816 | | 41.09 | , | | C |
| | ATOM | 16398 | | 2 TRP C 277 | | | | 35.159 | | 42.82 | | | C |
| | MOTA | 16399 | | 2 TRP C 277 | | 35.803 | 29.931 | | | 43.92 | | | c |
| .55 | MOTA | 16400 | | 3 TRP C 277 | | 35.193 | 29.196 | 36.190 | | | | | C |
| | MOTA | 16402 | | 3 TRP C 277 | | 35.938 | 28.193 | 36.833 | | 34.69 | | | C |
| | ATOM | | | 2 TRP C 277 | | 37.274 | 27.915 | | | 31.59 | | | |
| | MOTA | 16406 | CZ | 2 TRP C 277 | | 37.888 | 28.619 | 35.454 | | 28.84 | | | C |
| | ATOM | 16408 | С | TRP C 277 | | 31.559 | | | | 50.14 | | | C |
| 60 | ATOM | | 0 | TRP C 277 | | 30.821 | 31.528 | | | 53.55 | | | 0 |
| | MOTA | | | ASN C 278 | | 31.287 | 32.633 | 33.120 | 1.00 | 53.60 | | | N |
| | | | | • | | | | | | | | | |

| _ | | | | | | 22 561 | 22 272 | 1 00 50 74 | С |
|-----|-------|--------|-----|-----------|--------|--------|--------|------------|-----|
| - 5 | MOŢA | 16412 | | ASN C 278 | 30.173 | 33.561 | 33.273 | 1.00 50.74 | |
| | ATOM | 16414 | CB | ASN C 278 | 30.280 | 34.662 | 32.191 | 1.00 54.60 | C |
| | MOTA | 16417 | CG | ASN C 278 | 29.472 | 34.370 | 30.928 | 1.00 57.61 | С |
| | MOTA | 16418 | OD1 | ASN C 278 | 28.305 | 34.753 | 30.826 | 1.00 62.78 | 0 |
| | ATOM | 16419 | | ASN C 278 | 30.101 | 33.723 | 29.951 | 1.00 50.67 | N |
| 10 | TATOM | 16422 | | ASN C 278 | 28.767 | 32.886 | 33.392 | 1.00 52.28 | С |
| 10 | | 16423 | | ASN C 278 | 27.865 | 33.415 | 34.082 | 1.00 46.13 | 0 |
| | ATOM | | | ILE C 279 | 28.582 | 31.714 | 32.777 | 1.00 52.83 | N |
| | ATOM | 16424 | N | | | 31.048 | 32.896 | 1.00 56.47 | C |
| | ATOM | 16426 | CA | ILE C 279 | 27.287 | 29.838 | 31.946 | 1.00 57.69 | . C |
| | ATOM | 16428 | CB | ILE C 279 | 27.104 | | | 1.00 57.27 | Č |
| 15 | ATOM | 16430 | | ILE C 279 | 27.859 | 28.617 | 32.471 | | Č |
| | MOTA | 16433 | | ILE C 279 | 27.534 | 27.307 | 31.703 | 1.00 54.35 | |
| | ATOM | 16437 | CG2 | ILE C 279 | 27.493 | 30.172 | 30.507 | 1.00 58.04 | C |
| | ATOM | 16441 | С | ILE C 279 | 27.047 | 30.544 | 34.300 | 1.00 57.88 | C |
| • | ATOM | 16442 | 0 | ILE C 279 | 25.936 | 30.141 | 34.610 | 1.00 59.87 | 0 |
| 20 | ATOM | 16443 | N | PHE C 280 | 28.078 | 30.544 | 35.144 | 1.00 56.99 | N |
| 20 | ATOM | 16445 | CA | PHE C 280 | 27.934 | 30.040 | 36.500 | 1.00 51.07 | С |
| | ATOM | 16447 | СВ | PHE C 280 | 29.142 | 29.215 | 36.869 | 1.00 54.92 | C |
| | | 16450 | CG | PHE C 280 | 29.180 | 27.861 | 36.227 | 1.00 51.56 | · C |
| | ATOM | | | PHE C 280 | 28.625 | 26.777 | 36.852 | 1.00 48.09 | . C |
| 05 | ATOM | 16451 | | | 28.675 | 25.583 | 36.298 | 1.00 46.71 | · c |
| 25 | MOTA | 16453 | | PHE C 280 | | | 35.110 | 1.00 53.19 | c |
| | MOTA | 16455 | CZ | PHE C 280 | 29.262 | 25.412 | | 1.00 52.26 | c |
| | ATOM | 16457 | | PHE C 280 | 29.822 | 26.462 | 34.471 | | Č |
| | MOTA | 16459 | CD2 | PHE C 280 | 29.781 | 27.683 | 35.031 | 1.00 48.92 | |
| | MOTA | 16461 | С | PHE C 280 | 27.888 | 31.203 | 37.432 | 1.00 48.27 | C |
| 30 | MOTA | 16462 | 0 | PHE C 280 | 28.646 | 32.139 | 37.277 | 1.00 47.19 | . 0 |
| | MOTA | 16463 | N | PRO C 281 | 27.031 | 31.141 | 38.427 | 1.00 45.62 | N |
| | ATOM | 16464 | CA. | PRO C 281 | 26.801 | 32.279 | 39.285 | 1.00 47.19 | C |
| | ATOM | 16466 | CB | PRO C 281 | 25.373 | 32.029 | 39.741 | 1.00 48.28 | С |
| - | ATOM | 16469 | CG | PRO C 281 | 25.269 | 30.542 | 39.864 | 1.00 44.59 | С |
| 35 | ATOM | 16472 | CD | PRO C 281 | 26.237 | 29.991 | 38.869 | 1.00 48.35 | C |
| 55 | MOTA | 16475 | C | PRO C 281 | 27.761 | 32.335 | 40.463 | 1.00 48.66 | С |
| | | 16476 | Ö | PRO C 281 | 28.525 | 31.410 | 40.674 | 1.00 56.99 | 0 |
| | ATOM | | N | VAL C 282 | 27.712 | 33.423 | 41.214 | 1.00 46.97 | · N |
| | ATOM | 16477 | | VAL C 282 | 28.597 | 33.628 | 42.345 | 1.00 44.44 | С |
| 40 | ATOM | 16479 | CA | | 29.071 | 35.020 | 42.430 | 1.00 44.57 | C |
| 40 | ATOM | 16481 | CB | VAL C 282 | | | 41.118 | 1.00 45.56 | c |
| | MOTA | 16483 | | VAL C 282 | 29.756 | 35.469 | | 1.00 34.25 | Ċ |
| | ATOM | 16487 | | VAL C 282 | 27.890 | 36.003 | 42.759 | | Č |
| | MOTA | 16491 | С | VAL C 282 | 27.739 | 33.349 | 43.545 | 1.00 45.50 | o |
| | MOTA | 16492 | 0 | VAL C 282 | 26.506 | 33.444 | 43.451 | 1.00 42.57 | |
| 45 | MOTA | 16493 | N | ILE C 283 | 28.375 | 33.027 | 44.664 | 1.00 38.05 | N |
| | ATOM | .16495 | CA | ILE C 283 | 27.636 | 32.624 | 45.821 | 1.00 39.60 | - C |
| | MOTA | 16497 | CB | ILE C 283 | 27.997 | 31.210 | 46.205 | 1.00 42.77 | C |
| • | ATOM | 16499 | CG1 | ILE C 283 | 27.296 | 30.218 | 45.282 | 1.00 45.31 | . C |
| | ATOM | 16502 | CD1 | ILE C 283 | 28.010 | 28.859 | 45.202 | 1.00 51.32 | . С |
| 50 | ATOM | 16506 | | ILE C 283 | 27.494 | 30.935 | 47.573 | 1.00 48.65 | C |
| 50 | ATOM | 16510 | C | ILE C 283 | 27.951 | | 46.938 | 1.00 36.72 | С |
| | | 16511 | ŏ | ILE C 283 | 29.060 | 33.947 | 47.071 | 1.00 39.41 | 0 |
| | MOTA | | | SER C 284 | 26.964 | 33.814 | 47.765 | 1.00 43.61 | · N |
| | MOTA | 16512 | N | | | 34.724 | 48.883 | 1.00 42.34 | C |
| | MOTA | 16514 | CA | SER C 284 | 27.196 | | | | c |
| 55 | ATOM | 16516 | CB | SER C 284 | 26.479 | | 48.680 | 1.00 40.69 | |
| | MOTA | 16519 | OG | SER C 284 | 26.967 | | 47.532 | 1.00 40.19 | 0 |
| | ATOM | 16521 | С | SER C 284 | 26.765 | | 50.197 | 1.00 42.31 | c |
| | MOTA | 16522 | 0 | SER C 284 | 25.721 | | | 1.00 42.00 | 0 |
| | ATOM | 16523 | N | LEU C 285 | 27.605 | | 51.159 | | N |
| 60 | ATOM | 16525 | CA | LEU C 285 | 27.239 | 33.946 | 52.450 | | c |
| | ATOM | 16527 | СВ | LEU C 285 | 28.263 | | 52.951 | 1.00 43.13 | C |
| | | | | | | | | | |

| 5 | ATOM | 16530 | CG | LEU C 28 | 35 | 28.493 | 31.677 | 52.107 | 1.00 | 43.50 | | | С |
|----|--------------|----------------|---------|----------|-----|------------------|------------------|------------------|------|----------------|---|---|--------|
| • | ATOM | 16532 | | LEU C 28 | | 29.160 | 30.630 | 52.986 | 1.00 | 45.83 | | | C |
| | MOTA | 16536 | | LEU C 28 | | 27.224 | 31.096 | 51.550 | | 47.33 | | | С |
| | ATOM | 16540 | С | LEU C 28 | 85 | 27.238 | 35.237 | 53.241 | | 38.54 | | | С |
| | ATOM | 16541 | 0 | LEU C 28 | 85 | 28.192 | 36.012 | 53.142 | | 38.71 | | | 0 |
| 10 | ATOM | 16542 | N | TYR C 28 | 86 | 26.182 | 35.508 | 54.004 | | 41.40 | | | N |
| | ATOM | 16544 | CA | TYR C 28 | 86 | 26.201 | 36.697 | 54.882 | | 43.34 | | | С |
| | ATOM | 16546 | CB | TYR C 28 | 86 | 24.868 | 37.456 | 54.919 | | 43.01 | | | С |
| | MOTA | 16549 | ĆG | TYR C 28 | 86 | 24.458 | 38.178 | 53.648 | | 43.98 | _ | | С |
| | ATOM | 16550 | CD1 | TYR C 2 | 86 | 24.169 | 37.480 | 52.485 | | 41.24 | | | С |
| 15 | MOTA | 16552 | CE1 | TYR C 2 | 86 | 23.796 | 38.118 | 51.350 | | 37.43 | | | C |
| | MOTA | 16554 | CZ | TYR C 2 | | 23.683 | 39.479 | 51.318 | | 38.55 | | | C |
| | ATOM | 16555 | OH | TYR C 2 | | | 40.098 | 50.129 | | 31.80 | | | 0 |
| | ATOM | 16557 | | TYR C 2 | | 23.950 | 40.197 | 52.451 | | 36.26 | | | Ċ |
| - | ATOM | 16559 | CD2 | TYR C 2 | | 24.331 | 39.541 | 53.615 | | 41.46 | | | C |
| 20 | ATOM | 16561 | С | TYR C 2 | | 26.525 | 36.179 | 56.278 | | 40.55 | • | | C |
| | ATOM | 16562 | 0 | TYR C 2 | | 25.810 | 35.340 | 56.792 | | 35.99 | | | 0 |
| | ATOM | 16563 | N | LEU C 2 | | 27.609 | 36.668 | 56.876 | | 43.12 | | | N C |
| - | MOTA | 16565 | CA | LEU C 2 | | 27.992 | 36.203 | 58.201 | | 44.11 | | | |
| | MOTA | 16567 | CB | LEU C 2 | | 29.451 | 35.807 | 58.319 | | 44.04 | | | C C |
| 25 | MOTA | 16570 | CG | LEU C 2 | | 30.022 | 34.821 | 57.316 | | 45.36 | | | C |
| | MOTA | 16572 | | LEU C 2 | | 31.494 | 35.117 | 57.164 | | 48.19 | | | C |
| | ATOM | 16576 | | LEU C 2 | | 29.854 | 33.410 | 57.786 | | 49.68 | | | C |
| | MOTA | 16580 | С | LEU C 2 | | 27.750 | 37.322 | 59.116 | | 41.05 45.70 | | | o |
| | MOTA | 16581 | 0 | LEU C 2 | | 27.724 | 38.435 | 58.705 | | 48.49 | | | N |
| 30 | MOTA | 16582 | N | MET C 2 | | 27.578 | 36.981 | 60.370 61.414 | | 50.98 | | | C |
| | MOTA | 16584 | CA | MET C 2 | | 27.201 | 37.884 | 62.614 | | 53.16 | | | c |
| | MOTA | 16586 | CB | MET C 2 | | 26.743 | 37.033 37.824 | | | 59.82 | | | Ċ |
| | ATOM | 16589 | ĊG | MET C 2 | | 26.255 | 36.852 | 65.181 | | 66.84 | | • | s |
| 26 | ATOM | 16592 | SD | MET C 2 | | 25.588 24.400 | 35.852 | 64.340 | | 65.00 | | | č |
| 35 | MOTA | 16593 | CE | MET C 2 | | 28.448 | 38.645 | 61.724 | | 52.60 | | | c |
| | ATOM | 16597 | c | MET C 2 | | 29.541 | 38.109 | 61.660 | | 49.84 | | | ō |
| | MOTA | 16598 | O N | GLY C 2 | | 28.298 | 39.906 | 62.056 | | 53.80 | • | | N |
| | ATOM | 16599 | N CA | GLY C 2 | | | 40.726 | 62.323 | | 53.77 | | | C |
| 40 | ATOM ATOM | 16601 16604 | CA | GLY C 2 | | 29.552 | 41.029 | 63.794 | | 52.86 | • | | Ċ |
| 40 | ATOM | 16605 | o | GLY C 2 | | 28.759 | 40.561 | 64.560 | | 55.64 | | | 0 |
| | ATOM | 16606 | N | GLU C 2 | | 30.527 | 41.828 | 64.185 | | 59.63 | | | N. |
| | ATOM | 16608 | CA | GLU C 2 | 90 | 30.713 | 42.194 | 65.586 | | 62.62 | | | C |
| | ATOM | 16610 | CB | GLU C 2 | | 32.131 | 42.676 | 65.770 | | 61.72 | | | С |
| 45 | MOTA | 16613 | CG | GLU C 2 | | 33.118 | 41.620 | 65.403 | 1.00 | 56.49 | | | С |
| .5 | ATOM | 16616 | CD | GLU C 2 | | 34.316 | | 66.263 | 1.00 | 62.75 | | | C |
| | ATOM | 16617 | | GLU C 2 | | 35.173 | 42.598 | 65.952 | | 66.45 | | | 0 |
| | ATOM | 16618 | | GLU C 2 | | 34.368 | 40.951 | 67.245 | 1.00 | 58.63 | | | 0 |
| | ATOM | 16619 | C | GLU C 2 | 290 | 29.799 | 43.253 | 66.185 | | 66.84 | | | С |
| 50 | ATOM | 16620 | 0 | GLU C 2 | | 29.553 | 43.241 | 67.411 | 1.00 | 65.72 | | | 0 |
| | MOTA | 16621 | N | VAL C 2 | | 29.309 | 44.171 | 65.356 | 1.00 | 71.13 | | | N |
| | ATOM | 16623 | CA | VAL C 2 | | 28.433 | 45.221 | 65.869 | 1.00 | 74.55 | | | С |
| | ATOM | 16625 | CB | VAL C 2 | 291 | 28.539 | 46.525 | 65.086 | | 76.24 | | | С |
| | ATOM | 16627 | CG1 | VAL C 2 | | 27.577 | 47.563 | 65.658 | 1.00 | 76.47 | | | C |
| 55 | ATOM | 16631 | | VAL C 2 | | 29.953 | 47.059 | | | 81.20 | | | С |
| | MOTA | 16635 | С | VAL C 2 | | 27.003 | 44.778 | 65.840 | | 75.19 | | | C |
| | ATOM | 16636 | 0 | VAL C 2 | | 26.553 | 44.138 | 64.875 | | 76.87 | | | . 0 |
| | MOTA | 16637 | N | THR C 2 | | 26.299 | | | | 76.63 | | | N |
| | MOTA | | CA | THR C 2 | | 24.884 | 44.803 | 67.090 | | 78.73 | | | C |
| 60 | ATOM | 16641 | CB | THR C 2 | | 24.380 | | | | 79.80 | | | C |
| | MOTA | 16643 | OG1 | THR C 2 | 292 | 25.508 | 46.083 | 69.035 | 1.00 | 83.48 | | | 0 |

| 5 | MOTA | 16645 | CG2 | THR C 292 | | 23.660 | 44.683 | 69.301 | 1.00 | 82.75 | | | С |
|-----|------|--------|-----|-------------|----|--------|--------|--------|------|---------|---|---|-----|
| , | ATOM | 16649 | | THR C 292 | | 24.039 | 45.118 | 65.842 | 1.00 | 78.20 | | | С |
| - | ATOM | 16650 | | THR C 292 | | 24.152 | 46.206 | 65.281 | 1.00 | 76.52 | | | 0 |
| • | | 16651 | | GLN C 293 | | 23.212 | 44.153 | 65.414 | 1.00 | 77.10 | | | N |
| | ATOM | | | GLN C 293 | | 22.352 | 44.280 | 64.223 | | 73.84 | | | С |
| | MOTA | 16653 | | | | 21.520 | 45.562 | 64.352 | | 79.00 | | | С |
| 10 | ATOM | 16655 | | GLN C 293 | | | 45.347 | 64.881 | | 85.11 | | | С |
| | ATOM | 16658 | | GLN C 293 | | 20.073 | | 66.165 | | 87.31 | | | c |
| | ATOM | 16661 | | GLN C 293 | | 19.749 | 46.139 | | | 85.12 | | , | ő |
| | MOTA | 16662 | | GLN C 293 | | 18.960 | 45.672 | 67.007 | | | • | | N |
| | MOTA | 16663 | | GLN C 293 | | 20.347 | 47.329 | 66.308 | | 86.21 | | | Č |
| 15 | ATOM | 16666 | С | GLN C 293 | | 23.045 | 44.268 | 62.842 | | 65.85 | | - | |
| | ATOM | 16667 | 0 | GLN C 293 | | 22.370 | 44.359 | 61.822 | | 63.96 | | | 0 |
| | MOTA | 16668 | N | GLN C 294 | • | 24.366 | 44.120 | 62.803 | | 66.61 | | | N |
| | ATOM | 16670 | CA | GLN C 294 | | 25.141 | 44.364 | 61.580 | | 61.35 | | | С |
| • | ATOM | 16672 | СВ | GLN C 294 | | 26.324 | 45.288 | 61.936 | 1.00 | 60.41 | | | С |
| 20 | ATOM | 16675 | CG | GLN C 294 | | 26.837 | 46.202 | 60.839 | 1.00 | 62.21 | | | С |
| 20 | | 16678 | | GLN C 294 | | 27.669 | 47.413 | 61.365 | 1.00 | 65.59 | | | С |
| | ATOM | | | GLN C 294 | | 28.765 | 47.713 | 60.847 | | 59.99 | | | 0 |
| | MOTA | 16679 | | GLN C 294 | | 27.138 | 48.107 | 62.373 | | 65.49 | | | N |
| | ATOM | 16680 | | | | 25.627 | 43.036 | 60.985 | | 56.94 | | | С |
| | ATOM | 16683 | C | GLN C 294 | | | 42.085 | 61.710 | | 58.82 | | | ō |
| 25 | MOTA | 16684 | 0 | GLN C 294 | | 25.912 | | | | 46.60 | | | Ŋ |
| • | MOTA | 16685 | N | SER C 295 | | 25.718 | 42.958 | 59.668 | | | | | Ċ |
| | MOTA | 16687 | CA | SER C 295 | | 26.213 | 41.760 | 59.056 | | 42.55 | | | C. |
| | ATOM | 16689 | CB | SER C 295 | | 25.079 | 40.909 | 58.628 | | 40.84 | | | |
| | ATOM | 16692 | OG | SER C 295 | | 24.697 | 41.439 | 57.411 | | 43.82 | | | 0 |
| 30 | ATOM | 16694 | С | SER C 295 | | 26.965 | 42.103 | 57.806 | | 44.01 | | | Ċ |
| | ATOM | 16695 | 0 | SER C 295 | | 26.877 | 43.217 | 57.316 | | 41.78 | • | | 0 |
| | ATOM | 16696 | N | PHE C 296 | | 27.688 | 41.133 | 57.260 | | 40.42 | • | | N |
| | ATOM | 16698 | CA | PHE C 296 | ٠. | 28.455 | 41.395 | 56.077 | 1.00 | 40.53 | | | C |
| | ATOM | 16700 | СВ | PHE C 296 | | 29.870 | 41.876 | 56.413 | 1.00 | 42.71 | | | . С |
| 35 | ATOM | 16703 | CG | PHE C 296 | | 30.782 | 40.825 | 56.974 | 1.00 | 40.05 | | | C |
| 33 | | 16704 | | PHE C 296 | | 31.588 | 40.081 | 56.147 | 1.00 | 43.51 | | | С |
| | MOTA | 16704 | | PHE C 296 | | 32.406 | 39.148 | 56.647 | | 36.06 | | | C |
| | ATOM | | CZ | PHE C 296 | | 32.443 | 38.940 | 58.011 | | 42.47 | | | С |
| | ATOM | 16708 | | PHE C 296 | | 31.674 | 39.657 | 58.822 | | 37.71 | | | С |
| 40 | MOTA | 16710 | | PHE C 296 | | 30.848 | 40.602 | 58.315 | | 37.78 | | | С |
| 40 | ATOM | 16712 | | | | 28.455 | 40.127 | 55.332 | | 42.08 | | | С |
| | MOTA | 16714 | C | PHE C 296 | | | | 55.906 | | 46.21 | | | 0 |
| | ATOM | 16715 | 0 | PHE C 296 | | 28.030 | 39.122 | | | 40.78 | | | N |
| | MOTA | 16716 | N | ARG C 297 | | 28.908 | 40.167 | 54.070 | | | | | c |
| | MOTA | 16718 | CA | ARG C 297 | | 28.958 | 38.974 | 53.211 | | 44.56 | | | Č |
| 45 | MOTA | 1,6720 | CB | ARG C 297 | | 27.894 | 39.031 | 52.123 | | 44.33 | | | C |
| | MOTA | 16723 | CG. | ARG C 297 | | 28.197 | 40.056 | 51.064 | | 50.40 | | | |
| | ATOM | 16726 | CD | ARG C 297 | | 27.009 | 40.427 | 50.181 | | 54.77 | | | ~ C |
| | ATOM | 16729 | NE | ARG C 297 | | 27.370 | 41.445 | 49.195 | | 56.04 | | | N |
| | ATOM | 16731 | CZ | ARG C 297 | | 26.505 | 42.187 | 48.535 | | 50.69 | | | C |
| 50 | ATOM | 16732 | | ARG C 297 | | 25.204 | 42.040 | 48.732 | 1.00 | 51.47 | | | N |
| 50 | ATOM | 16735 | | ARG C 297 | | 26.946 | 43.079 | 47.677 | 1.0 | 0 46.53 | | | N |
| | ATOM | 16738 | С | ARG C 297 | | 30.273 | | 52.498 | 1.0 | 0 42.25 | | | С |
| | | | Ö | ARG C 297 | | 31.035 | | 52.215 | | 0.47.66 | | | 0 |
| | ATOM | | | ILE C 298 | | 30.518 | | 52.194 | | 0 41.06 | | | N |
| ~ ~ | ATOM | 16740 | N | | | 31.679 | | 51.439 | | 0 41.71 | | | C |
| 55 | ATOM | 16742 | CA | ILE C 298 | | | | 52.264 | | 0 38.04 | | | Ċ |
| • | ATOM | | CB | ILE C 298 | | 32.517 | | 52.204 | | 0 39.04 | | | Č |
| | MOTA | | | ILE C 298 | | 31.858 | | | | | | | c |
| | MOTA | | | ILE C 298 | | 32.459 | | 53.357 | | 0 42.84 | | | C |
| | ATOM | | | 2 ILE C 298 | | 32.654 | | 53.672 | | 0 37.72 | | | C |
| 60 | ATOM | 16757 | С | ILE C 298 | | 31.051 | | | | 0 36.43 | | | |
| | ATOM | | 0 | ILE C 298 | | 29.989 | 35.993 | 50.268 | 1.0 | 0 39.29 | | | 0 |
| | | | | | | | | | | | | | |

| | | <u>.</u> | | | | | | | | | |
|------|------|----------|------|-------|--------|-----------|--------|--------|--------|------------|-----|
| 5 | ATOM | 16759 | N · | THR C | 299 | | 31.675 | 36.727 | 49.041 | 1.00 41.37 | N |
| | ATOM | 16761 | CA | THR C | 299 | | 31.098 | 36.225 | 47.769 | 1.00 42.98 | С |
| | MOTA | 16763 | CB | THR C | 299 | | 30.626 | 37.411 | 46.893 | 1.00 44.37 | С |
| | MOTA | 16765 | OG1 | THR C | 299 | | 30.064 | 38.411 | 47.749 | 1.00 48.01 | 0 |
| | ATOM | 16767 | | THR C | | • | 29.455 | 37.062 | 45.991 | 1.00 45.15 | |
| 10 | | 16771 | | THR C | | | 32.163 | 35.478 | 47.050 | 1.00 38.51 | С |
| 10 | MOTA | | | THR C | | | 33.282 | 35.947 | 46.931 | 1.00 38.31 | 0 - |
| | ATOM | 16772 | | | | | | | 46.557 | 1.00 40.54 | |
| | ATOM | 16773 | N | ILE C | | | 31.834 | 34.309 | | 1.00 40.34 | |
| | MOTA | 16775 | .CA | ILE C | | | 32.849 | 33.494 | 45.920 | | |
| | MOTA | 16777 | CB | ILE (| | | 33.019 | 32.177 | 46.685 | 1.00 40.87 | |
| 15 | MOTA | 16779 | CG1 | ILE C | 300 | | 32.051 | 31.162 | 46.204 | 1.00 34.13 | |
| | ATOM | 16782 | CDI | ILE C | 300 | | 32.254 | 29.851 | 46.922 | 1.00 36.30 | |
| | ATOM | 16786 | CG2 | ILE (| 300 | | 32.721 | 32.317 | 48.186 | 1.00 44.16 | |
| | ATOM | 16790 | | | 300 | · · · · · | 32.440 | 33.216 | 44.505 | 1.00 40.76 | C |
| • | ATOM | 16791 | | | 300 | | 31.254 | 33.277 | 44.220 | 1.00 39.41 | . 0 |
| 20 | | | | TEA (| | | 33.426 | 32.905 | 43.645 | 1.00 44.04 | |
| 20 | ATOM | 16792 | N | | | | | 32.633 | 42.210 | 1.00 45.48 | |
| | ATOM | 16794 | CA | LEU (| | | 33.215 | | | 1.00 47.46 | |
| | MOTA | 16796 | CB | TEO (| | | 34.199 | 33.429 | 41.340 | | |
| | ATOM | 16799 | CG | TEA (| 301 | | 34.544 | 34.876 | 41.679 | 1.00 50.30 | |
| | MOTA | 16801 | CD1 | LEU (| 301 | | 35.649 | 35.402 | 40.734 | 1.00 51.91 | |
| 25 | ATOM | 16805 | CD2 | LEU (| 301 | | 33.312 | 35.727 | 41.580 | 1.00 48.11 | |
| | ATOM | 16809 | С | LEU (| | | 33.338 | 31.183 | 41.734 | 1.00 46.00 | C |
| | ATOM | 16810 | ō | | 301 | | 33.844 | 30.283 | 42.386 | 1.00 40.23 | 0 |
| | | 16811 | N | | 302 | | 32.905 | 30.973 | 40.516 | 1.00 47.02 | N |
| | ATOM | | | | 302 | | 32.898 | 29.626 | 39.965 | 1.00 45.68 | |
| 20 | MOTA | 16812 | CA | | | | 32.276 | 29.806 | 38.584 | 1.00 43.48 | |
| 30 | ATOM | 16814 | CB | | 302 | | | | 38.541 | 1.00 45.27 | |
| | ATOM | 16817 | CG | | 302 | | 31.796 | 31.181 | | | |
| | ATOM | 16820 | CĐ | | 302 | | 32.456 | 31.994 | 39.567 | 1.00 42.09 | _ |
| | ATOM | 16823 | С | PRO (| 302 | | 34.331 | 29.104 | 39.891 | 1.00 48.54 | |
| | ATOM | 16824 | 0 | PRO (| C 302 | | 34:534 | 27.886 | 39.845 | 1.00 49.42 | |
| 35 | ATOM | 16825 | N | GLN (| C 303 | | 35.309 | 30.014 | 39.873 | 1.00 47.34 | |
| | ATOM | 16827 | CA | GLN (| C 303 | | 36.708 | 29.610 | 39.973 | 1.00 47.58 | |
| | ATOM | 16829 | СВ | | C 303 | | 37.637 | 30.790 | 39.736 | 1.00 47.37 | C |
| | ATOM | 16832 | CG | | C ·303 | | 37.910 | 31.131 | 38.293 | 1.00 45.62 | |
| | | 16835 | CD | | C 303 | | 36.936 | 32.113 | 37.717 | 1.00 45.06 | |
| 40 | ATOM | | | | C 303 | | 35.838 | 32.299 | 38.244 | 1.00 37.43 | |
| 40 | ATOM | 16836 | | | | | | 32.747 | 36,617 | 1.00 50.52 | |
| | ATOM | 16837 | | | C 303 | | 37.334 | | | | |
| | ATOM | 16840 | C | | C 303 | | 37.068 | 28.996 | 41.346 | 1.00 49.02 | |
| | ATOM | 16841 | 0 | | C 303 | | 38.159 | 28.473 | 41.514 | 1.00 51.60 | = |
| | ATOM | 16842 | N | GLN | C 304 | | 36.169 | 29.052 | 42.316 | 1.00 49.47 | |
| 45 | ATOM | 16844 | CA | GLN. | C 304 | | 36.438 | 28.475 | 43.616 | 1.00 50.38 | |
| | MOTA | 16846 | CB | GLN | C 304 | | 36.269 | 29.511 | 44.737 | 1.00 52.4 | |
| | ATOM | 16849 | CG | | C 304 | | 37.510 | 30.399 | 44.949 | 1.00 50.60 | 6 C |
| | ATOM | 16852 | · CD | | C 304 | | 37.438 | | 44.151 | 1.00 51.4 | 5 C |
| | | 16853 | | | C 304 | | 38.235 | 31.881 | 43.210 | 1.00 51.29 | |
| - ΕΛ | ATOM | | | | | | 36.484 | 32.532 | 44.509 | 1.00 40.5 | |
| 50 | ATOM | 16854 | | | C 304 | | | | | | |
| | ATOM | 16857 | С | | C 304 | | 35.606 | 27.249 | 43.939 | 1.00 51.9 | |
| | MOTA | 16858 | 0 | | C 304 | | 36.120 | | 44.554 | 1.00 55.4 | - |
| | MOTA | 16859 | N | | C-305 | | 34.328 | 27.212 | 43.574 | 1.00 56.2 | 9 N |
| | MOTA | 16861 | CA | TYR | C 305 | | 33.569 | 25.956 | 43.788 | 1.00 52.7 | |
| 55 | MOTA | 16863 | CB | TYR | C 305 | | 32.064 | 26.151 | 44.100 | 1.00 50.8 | 0 C |
| - | ATOM | 16866 | CG | | C 305 | | 31.206 | 26.929 | 43.131 | 1.00 44.8 | |
| | ATOM | 16867 | | | C 305 | | 30.417 | 26.271 | 42.212 | 1.00 44.8 | 8 C |
| | | 16869 | | | C 305 | | 29.642 | 26.928 | 41.352 | 1.00 35.0 | |
| | ATOM | | | | C 305 | | 29.594 | 28.271 | 41.368 | 1.00 36.8 | |
| 60 | ATOM | 16871 | | | | | | 28.910 | | | |
| 60 | ATOM | 16872 | OH | | C 305 | | 28.748 | | | | |
| | ATOM | 16874 | CE2 | TYR | C 305 | • | 30.352 | 28.964 | 42.269 | 1.00 37.2 | |

| | | | | | | | | | | the state of the s |
|------------|--------------|-------|----------|-------|-------|------|----------|----------|-------------|--|
| 5 | ATOM | 16876 | CD2 | TYR C | 305 | 31.1 | 49 28.29 | 0 43.155 | 1.00 38.7 | 8 C |
| _ | ATOM | 16878 | C. | TYR C | | 33.7 | | | | |
| | ATOM | 16879 | ō | TYR C | | 33.3 | | , | | |
| | ATOM | 16880 | N | LEU C | | 34.4 | | | | |
| | ATOM | 16882 | CA | LEU C | | 34.7 | | | | |
| 10 | ATOM | 16884 | СВ | LEU C | | 34.3 | | | | • |
| . 10 | ATOM | 16887 | CG | LEU C | | 32.9 | | 5 38.761 | | |
| | ATOM | 16889 | | LEU C | | 32.7 | | | | |
| | ATOM | 16893 | | LEU C | | 32.3 | | | | |
| | ATOM | 16897 | C | LEU C | | 36.1 | | | | |
| 15 | ATOM | 16898 | ō | TEO C | | 37.0 | | | | |
| 15 | ATOM | 16899 | N | ARG C | | 36.5 | | | | |
| | | 16901 | CA | ARG C | | 37.8 | | | | |
| | ATOM ATOM | 16903 | CB | ARG C | | 37.8 | | | | |
| | | 16906 | CG | ARG C | | 39.2 | | | | |
| 20 | ATOM | | | | | 39.2 | | | | |
| 20 | ATOM | 16909 | CD | ARG C | | 38.5 | • | | | |
| | ATOM | 16912 | NE CZ | | | | | | | |
| | ATOM | 16914 | CZ | ARG C | | 38.9 | : | | | |
| | ATOM | 16915 | | ARG C | | 40.0 | | | | |
| 25 | ATOM | 16918 | | ARG C | | 38.2 | | | | |
| 25 | ATOM | 16921 | C | ARG C | | 38.6 | | | | |
| • | ATOM | 16922 | 0 | ARG C | | 38.1 | | | | |
| | ATOM | 16923 | N | PRO C | | 39.7 | | | | - |
| • | ATOM | 16924 | CA | PRO C | | 40.5 | | | | |
| 20 | MOTA | 16926 | CB | PRO C | | 41.6 | | | | |
| 30 | ATOM | 16929 | CG | PRO C | | 41.3 | | | | |
| | MOTA | 16932 | ĆĐ | PRO C | | 40.3 | | | | |
| | ATOM | 16935 | С | PRO C | | 41.2 | | | | |
| • | ATOM. | 16936 | 0 | PRO C | | 41.8 | | • | | |
| 25 | ATOM | 16937 | N | VAL C | | 41.0 | | | | |
| 35 | ATOM | 16939 | CA | VAL C | | 41.6 | | | | |
| • | ATOM | 16941 | | VAL C | | 40.5 | | | | |
| | ATOM | 16943 | | VAL C | | 39.5 | | | | |
| | ATOM | 16947 | | VAL C | | 39.7 | | | | |
| 40 | MOTA | 16951 | C | VAL C | | 42.3 | | | | |
| 40 | MOTA | 16952 | 0 | VAL C | | | | | | |
| • | MOTA | 16953 | N | GLU C | | 42.6 | | | | |
| | ATOM | 16955 | CA | GLU C | | 43.2 | | | | |
| | ATOM | 16957 | CB | | | 44.3 | | | | |
| 45 | ATOM | 16960 | CG | GLU C | | 45.6 | | | | |
| 42 | ATOM | 16963 | CD | GLU C | | 45.5 | | | | |
| | ATOM | 16964 | | | | 45.1 | | | | |
| • | ATOM | 16965 | | GLU C | | 45.9 | . , | • | | |
| | ATOM | 16966 | C | | | 42.3 | | - | | |
| 50 | ATOM | 16967 | 0 | GLU C | | 41.7 | | | | |
| 50 | ATOM | 16968 | N | ASP C | | 42.0 | | | | |
| | ATOM | 16970 | CA | ASP C | | | | | | |
| | ATOM | 16972 | CB | ASP C | | 41.2 | | | | |
| • | ATOM | 16975 | CG | ASP C | | 40.4 | | | | |
| | ATOM | 16976 | | ASP C | | 40.0 | | | | |
| 55 | ATOM | 16977 | | ASP C | | 40.1 | | | | |
| • | ATOM | 16978 | С | ASP C | | 41.7 | | | | |
| | ATOM | 16979 | 0 | ASP C | | 42.9 | | | | |
| | ATOM | 16980 | N | VAL C | | 40.8 | | | | |
| <i>(</i> 0 | ATOM | 16982 | CA | VAL C | | 41.1 | | | | |
| 60 | ATOM | 16984 | CB | VAL C | | 39.9 | | | | - |
| | ATOM | 16986 | CG1 | VAL C | . 312 | 40.2 | 264 8.3 | 48 32.29 | 0 1.00102.6 | . C |
| | | | | | | | | | • | |

```
16990 CG2 VAL C 312
 5 ATOM
                                         38.650 10.202 32.861 1.00100.40
     MOTA
            16994
                    С
                        VAL C 312
                                         42.428 10.292 31.906 1.00101.68
                        VAL C 312
     MOTA
            16995
                   0
                                         43.435
                                                   9.972 32.560 1.00102.27
     MOTA
            16996 N
                        ALA C 313
                                         42.397 10.320 30.571
                                                                    1.00 99.43
     ATOM
            16998
                        ALA C 313
                                         43.564
                                                  9.986 29.760
                                                                    1.00 96.81
                   CA
                        ALA C 313
10
     MOTA
            17000
                   CB
                                         43.127
                                                  9.454 28.395
                                                                    1.00 95.91
                                                                    1.00 96.79
     ATOM
                        ALA C 313
                                         44.444 11.222 29.625
            17004
                    С
     MOTA
            17005
                        ALA C 313
                                         45.096 11.442 28.606
                    0
                                                                    1.00 98.26
                         THR C 314
     ATOM
            17006
                    N
                                         44.434 12.009
                                                           30.703
                                                                    1.00 97.05
                                                                                            N
                        THR C 314
     MOTA
            17008
                    CA
                                         45.147
                                                  13.297
                                                           30.885
                                                                    1.00 96.61
                                                                                            С
                        THR C 314
15
     ATOM
                                         46.635 12.993
            17010
                    CB ·
                                                           31.175
                                                                    1.00 95.85
                                                                                            C
                    OG1 THR C 314
     ATOM
            17012
                                         47.210 12.241
                                                           30.101
                                                                    1.00 94.24
                                                                                            0
     ATOM
            17014
                    CG2 THR C 314
                                         46.755 12.067
                                                           32.397
                                                                    1.00 97.66
                        THR C 314
     ATOM
            17018
                                         45.031 14.507 29.891
                                                                    1.00 97.32
                    С
                                      45.031 14.507
45.827 15.447
44.056 14.526
43.911 15.601
42.513 15.511
42.361 16.442
44.158 17.114
                        THR C 314
     MOTA
            17019
                    0
                                         45.827 15.447 29.999
                                                                    1.00 99.24
20
                                         44.056 14.526 28.976 1.00 94.94
     MOTA
            17020
                    N
                        SER C 315
                                                                                            N
     MOTA
            17022
                        SER C 315
                                                           27.933
                                                                    1.00 94.95
                    CA
                                                                                            С
           17024 CB
     ATOM
                       SER C 315
                                                           27.298
                                                                    1.00 94.81
                                                                                            С
     ATOM 17027
                   OG
                        SER C 315
                                                           26.233
                                                                    1.00 93.24
                                                                                            0
     ATOM 17029
                        SER C 315
                                      44.158 17.114 28.237 1.00 93.29
44.341 17.532 29.385 1.00 90.39
                   C, ·
25
     ATOM 17030
                        SER C 315
                                     44.341 17.532 29.385 1.00 90.39

44.140 17.903 27.154 1.00 92.77

44.289 19.362 27.190 1.00 93.00

45.171 19.847 26.011 1.00 91.78

46.679 19.416 26.098 1.00 93.54

47.522 19.699 24.810 1.00 93.70

47.456 20.789 24.226 1.00 91.79

48.314 18.712 24.392 1.00 88.27
                   0
                   N
     ATOM
            17031
                        GLN C 316
                                                                                            N
     MOTA
            17033
                    CA
                        GLN C 316
                                                                                            C
     ATOM
            17035
                        GLN C 316
                    CB
                                                                                            C
                   CG GLN C 316
CD GLN C 316
OE1 GLN C 316
     ATOM
            17038
                                                                                           · C
30
            17041
     MOTA
                                                                                            C
     MOTA
           17042
                                                                                            0
                                     48.314 18.712

42.911 20.123

42.855 21.333

41.813 19.414

40.545 20.057

39.341 19.120

39.375 18.237

39.976 18.629

38.806 17.125

40.650 20.378

41.068 19.527
                   NE2 GLN C 316
     ATOM 17043
     ATOM 17046
                        GLN C 316
                                                           27.252
                    С
                                                                    1.00 92.97
     ATOM 17047
                        GLN C 316
                                                  21.333 27.012 1.00 97.12
                    0
35
     ATOM 17048
                        ASP C 317
                   N
                                                           27.541 1.00 88.86
     ATOM 17050
                        ASP C 317
                                                           27.925 1.00 85.72
                   ·CA
                                                                                            С
     ATOM 17052
                        ASP C 317
                    CB
                                                          27.813 1.00 89.42
                                                                                            C
     ATOM 17055
                    CG
                        ASP C 317
                                                           26.588 1.00 93.20
                                                                                            C
                    OD1 ASP C 317
            17056
     MOTA
                                                           25.560 1.00 97.12
                                                                                            0
40
     MOTA
            17057
                    OD2 ASP C 317
                                                           26.583 1.00 93.67
                                                                                            0
                                                           29.414 1.00 81.00
     ATOM
            17058
                    С
                        ASP C 317
                                                                                            С
                        ASP C 317
            17059
     ATOM
                    0
                                         41.068
                                                  19.527
                                                           30.190 1.00 76.59
                                                                                            O
                        ASP C 318
           17060
     MOTA
                                         40.260
                                                  21.571
                    N
                                                           29.843
                                                                    1.00 76.29
                                                                                            N
                    CA ASP C 318
     MOTA
           17062
                                         40.389 21.894
                                                           31.257
                                                                    1.00 69.79
                                      40.429 23.405
45
     ATOM
           17064
                       ASP C 318
                    CB
                                                           31.434
                                                                    1.00 70.73
                                      41.656 24.001
                                                                   1.00 75.33
     MOTA
            17067
                    CG ASP C 318
                                                           30.798
                                                                                            С
     ATOM
            17068
                    OD1 ASP C 318
                                       41.776 25.257
                                                           30.699 1.00 80.77
                                                                                            ·O
     ATOM
           17069
                                        42.561 23.260
                                                           30.360 1.00 79.35
                   OD2 ASP C 318
                                                                                            0
           17070
     MOTA
                   С
                        ASP C 318
                                         39.268 21.199
                                                           32.037
                                                                    1.00 63.07
                                                                                            C
50
     ATOM
            17071
                        ASP C 318
                   0
                                         38.103 21.409
                                                           31.755 1.00 54.32
                                                                                            0
     MOTA
            17072
                   N
                        CYS C 319
                                         39.624 20.356
                                                           33.005 1.00 61.35
                   CA CYS C 319
     MOTA
            17074
                                         38.611 19.604
                                                           33.753 1.00 62.73
                                         39.002 18.138
     MOTA
            17076
                   CB
                        CYS C 319
                                                           33.789 1.00 67.00
                                                                                           ·C
                                                 17.347
            17079
                        CYS C 319
     ATOM
                   SG
                                         39.025
                                                           32.147 1.00 71.83
                                                                                            S
55
                        CYS C 319
CYS C 319
     ATOM
           17080
                   .C
                                         38.309
                                                  20.122
                                                           35.176 1.00 60.27
                                                                                            C
           17081
                   Ο.
     MOTA
                                         39.157
                                                  20.741
                                                           35.825
                                                                    1.00 57.82
                                                                                            O
                        TYR C 320
     MOTA
           17082
                                         37.089 19.870
                   N
                                                           35.652
                                                                    1.00 53.68
                                                                                            N
     ATOM
            17084
                        TYR C 320
                                         36.675
                                                  20.393
                   CA
                                                           36.939
                                                                    1.00 49.77
     ATOM
            17086
                   CB
                        TYR C 320
                                         35.945
                                                  21.709
                                                           36.677
                                                                    1.00 50.01
60
     ATOM
            17089
                        TYR C 320
                                         36.861
                    CG
                                                  22.674
                                                           35.958
                                                                   1.00 48.43
     MOTA
            17090
                    CD1 TYR C 320
                                         36.774
                                                  22.878
                                                           34.601 1.00 45.90
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| 5 | ATOM | 17092 | CE1 | TYR C 320 | 3 | 37.633 | 23.740 | 33.956 | 1.00 45.11 | | | C |
|-------------|--------------|-------|------------|-------------|---|------------------|--------|--------|------------|-----|---|----|
| - | ATOM | 17094 | CZ | TYR C 320 | 3 | 38.584 | 24.406 | 34.665 | 1.00 42.05 | | | С |
| | ATOM | 17095 | OH | TYR C 320 | 3 | 39.464 | 25.286 | | 1.00 41.52 | | | 0 |
| • | ATOM | 17097 | CE2 | TYR C 320 | 3 | 38.678 | 24.213 | 36.008 | 1.00 49.88 | | | С |
| | ATOM | 17099 | CD2 | TYR C 320 | | 37.824 | 23.357 | 36.645 | 1.00 48.03 | | | С |
| 10 | ATOM | 17101 | С | TYR C 320 | : | 35.796 | 19.427 | 37.713 | 1.00 50.65 | | | С |
| | ATOM | 17102 | 0 | TYR C 320 | | 35.243 | 18.517 | 37.104 | 1.00 50.64 | | | 0 |
| | ATOM | 17103 | N | LYS C 321 | | 35.681 | 19.611 | 39.042 | 1.00 48.99 | ı | | N |
| | ATOM | 17105 | CA | LYS C 321 | : | 34.718 | 18.851 | 39.874 | 1.00 48.57 | | | С |
| | ATOM | 17107 | СВ | LYS C 321 | | 35.394 | 17.846 | 40.803 | 1.00 51.22 | | | С |
| 15 | ATOM | 17110 | CG | LYS C 321 | : | 35.994 | 16.592 | 40.130 | 1.00 59.14 | | | С |
| • • | ATOM | 17113 | CD | LYS C 321 | : | 36.034 | 15.363 | 41.092 | 1.00 60.36 | | | С |
| | ATOM | 17116 | CE | LYS C 321 | | 36.528 | 14.083 | 40.379 | 1.00 61.02 | ? | • | С |
| | ATOM | 17119 | NZ | LYS C 321 | | 36.887 | 12.972 | 41.327 | 1.00 60.51 | | | N |
| - | ATOM | 17123 | C | LYS C 321 | | 33.894 | 19.787 | 40.756 | 1.00 43.89 |) | | С |
| 20 | ATOM | 17124 | ō | LYS C 321 | | 34.388 | 20.685 | 41.391 | 1.00 48.32 | ? | | 0 |
| LU | ATOM | 17125 | N | PHE C 322 | | 32.614 | 19.570 | 40.806 | 1.00 45.73 | L | | N |
| | ATOM | 17127 | CA | PHE C 322 | | 31.772 | 20.381 | 41.647 | 1.00 45.13 | Ļ | | C |
| | ATOM | 17129 | СВ | PHE C 322 | | 30.325 | 19.886 | 41.516 | 1.00 39.38 | 3 | | С |
| | ATOM | 17132 | CG | PHE C 322 | | 29.275 | 20.890 | 41.937 | 1.00 47.52 | 2 | | С |
| 25 | ATOM | 17133 | | PHE C 322 | | 29.280 | 22.186 | 41.454 | 1.00 52.42 | | | С |
| 23 | ATOM | 17135 | | PHE C 322 | | 28.318 | 23.066 | 41.839 | 1.00 46.38 | | | С |
| | ATOM | 17137 | CZ | PHE C 322 | | 27.334 | 22.671 | 42.708 | 1.00 41.89 | 5 . | | C. |
| | ATOM | 17137 | | PHE C 322 | | 27.315 | 21.436 | 43.176 | 1.00 38.9 | | • | С |
| - ' | ATOM | 17133 | | PHE C 322 | | 28.266 | 20.535 | 42.801 | 1.00 38.9 | | | С |
| 30 | ATOM | 17143 | C | PHE C 322 | | 32.331 | 20.143 | 43.041 | 1.00 46.5 | 6. | | С |
| 30 | | 17143 | o' | PHE C 322 | | 32.334 | 18.998 | 43.496 | 1.00 55.3 | | | 0 |
| | ATOM | 17145 | N | ALA C 323 | | 32.827 | 21.180 | 43.713 | 1.00 40.6 | | | N- |
| | MOTA | 17147 | CA | ALA C 323 | | 33.267 | 21.030 | 45.100 | 1.00 36.9 | | | С |
| | ATOM ATOM | 17147 | CB | ALA C 323 | | 34.573 | 21.721 | 45.298 | 1.00 40.4 | | - | C. |
| 35 . | | 17153 | C | ALA C 323 | ٠ | 32.266 | 21.542 | 46.125 | 1.00 36.5 | | | С |
| 33 . | ATOM ATOM | 17154 | 0 | ALA C 323 | | 32.636 | 22.208 | 47.080 | 1.00 37.2 | | | .0 |
| | ATOM | 17155 | N | ILE C 324 | | 30.989 | 21.267 | 45.943 | 1.00 37.3 | | | N |
| | ATOM | 17157 | CA | ILE C 324 | | 30.015 | 21.630 | 46.965 | 1.00 36.1 | | | С |
| • | ATOM | 17159 | CB | ILE C 324 | | 29.023 | 22.599 | 46.424 | 1.00 39.7 | | | С |
| 40 | ATOM | 17161 | | ILE C 324 | | 29.739 | 23.761 | 45.817 | 1.00 38.8 | 8 . | | С |
| 70 | ATOM | 17164 | | ILE C 324 | | 28.812 | 24.873 | 45.598 | 1.00 45.3 | 5 | | С |
| | ATOM | 17168 | | ILE C 324 | | 28.083 | 23.152 | | 1.00 42.7 | | | C |
| | ATOM | 17172 | C | ILE C 324 | | 29.353 | 20.321 | 47.267 | 1.00 41.5 | 2 | | С |
| | ATOM | 17173 | ŏ | ILE C 324 | | 29.381 | 19.453 | 46.389 | 1.00 48.2 | 9 | | 0 |
| 45 | ATOM | 17174 | N | SER C 325 | | 28.788 | 20.145 | 48.473 | 1.00 43.9 | | | N |
| 73 | ATOM | 17174 | CA | SER C 325 | | 28.161 | 18.864 | 48.868 | 1.00 44.0 | | | С |
| | ATOM | 17178 | CB | SER C 325 | | 29.154 | 17.696 | 48.881 | 1.00 45.5 | | | C. |
| | ATOM | 17181 | OG | SER C 325 | | | 18.073 | | 1.00 56.8 | | | 0 |
| | | 17183 | C | SER C 325 | | 27.410 | 18.846 | 50.181 | 1.00 49.4 | | | C |
| 50 | MOTA | 17184 | ŏ | SER C 325 | | 27.528 | 19.750 | 51.015 | 1.00 54.0 | | | 0 |
| 70 | | 17185 | N | GLN C 326 | | 26.624 | 17.786 | 50.339 | 1.00 55.3 | | | N |
| | ATOM | 17187 | CA | GLN C 326 | | 25.797 | 17.593 | 51.509 | 1.00 59.3 | | | C |
| • | ATOM | | CB | GLN C 326 | | 24.512 | 16.803 | 51.166 | 1.00 62.2 | | | С |
| | ATOM | 17189 | | GLN C 326 | | 24.703 | 15.342 | 50.735 | 1.00 66.3 | | | С |
| 55 | ATOM | 17192 | | GLN C 326 | | 23.421 | 14.731 | 50.154 | 1.00 73.3 | | | С |
| 55 | MOTA | 17195 | CD OF 1 | | | 23.421 | 14.751 | 50.899 | 1.00 75.4 | | | ŏ |
| | MOTA | 17196 | | GLN C 326 | | | 14.511 | 48.826 | 1.00 73.1 | | | N |
| | MOTA | 17197 | | 2 GLN C 326 | | 23.388 | 16.965 | 52.682 | | | | C |
| | ATOM | 17200 | С | GLN C 326 | | 26.568 27.603 | 16.287 | 52.522 | | | | ŏ |
| <i>(</i> 0 | MOTA | 17201 | 0 | GLN C 326 | | | | | | | | N |
| 60 | ATOM | 17202 | N | SER C 327 | | 26.017 | | 55.118 | | | | c |
| | MOTA | 17204 | CA | SER C 327 | | 26.599 | 16.804 | 22.110 | 1.00 30.0 | | | · |

```
17206
                                     27.625 17.830
                                                     55.574
                                                             1.00 59.51
     ATOM
                  CB
                      SER C 327
                      SER C 327
                                 27.685 17.900
                                                     57.003
                                                             1.00 64.04
     MOTA
           17209
                  OG
                                  25.482 16.698
     MOTA
           17211
                      SER C 327
                                                     56.153
                                                             1.00 58.47
                                    24.390 17.271
                      SER C 327
                                                     56.006
                                                             1.00 55.40
     ATOM
           17212
                  0
                                    25.771 15.949
                      SER C 328
                                                     57.197
                                                             1.00 56.87
           17213 N
     MOTA
                                                     58.242
10
           17215
                 CA
                      SER C 328
                                     24.812 15.697
                                                             1.00 55.69
    ATOM
                      SER C 328
                  CB
                                     24.601 14.209
                                                     58.396
                                                             1.00 56.03
     ATOM
           17217
                                                             1.00 57.06
                      SER C 328
                                     25.854
                                             13.578
           17220
                  OG
                                                     58.688
     ATOM
     MOTA
           17222
                  С
                      SER C 328
                                     25.423
                                             16.268
                                                     59.490
                                                             1.00 57.40
     MOTA
           17223
                  0
                      SER C 328
                                     24.834
                                             16.198
                                                     60.576
                                                             1.00 60.77
                                                                                   0
                      THR C 329
                                     26.615
                                             16.839
                                                             1.00 53.35
15
     ATOM
           17224
                  N
                                                     59.341
                                                                                   N
                      THR C 329
                                                             1.00 51.27
                                     27.213 17.541
                                                     60.450
                                                                                   C
     ATOM
           17226
                  CA
                      THR C 329
                                     28.454 16.818
                                                     .60.897
                                                             1.00 51.43
           17228
     MOTA
                  CB
                  OG1 THR C 329
                                     29.278
                                             16.560
                                                     59.768
                                                             1.00 42.60
     MOTA
           17230
                  CG2 THR C 329
                                     28.078
                                             15.427
                                                     61.365
                                                             1.00 56.80
     MOTA
           17232
                                     27.466 19.007
20
     ATOM
           17236
                      THR C 329
                                                     60.149
                                                             1.00 48.82
                  С
                      THR C 329
                                    28.537
                                             19.544
                                                     60.411 1.00 59.16
    ATOM
           17237
                  0 .
                                  26.450 19.642
     ATOM
           17238
                  N
                      GLY C 330
                                                     59.581
                                                             1.00 46.96
                                                                                 · N
                                                            1.00 34.71
                      GLY C 330
                                     26.372
                                             21.083
                                                     59.478
     MOTA
           17240
                  CA
                                                                                   C
                                             21.538
                                                            1.00 32.91
                      GLY C 330
                                     27.118
                                                     58.279
                                                                                   С
     MOTA
           17243
                  С
25
                                                             1.00 31.32
           17244
                      GLY C 330
                                     27.478 20.707
                                                     57.498
                                                                                   0
     MOTA
                  0
                      THR C 331
                                     27.331
                                             22.847
                                                     58.173
                                                             1.00 38.41
           17245
                                                                                   N
     MOTA
                  N
                      THR C 331
                                     28.081
                                             23.522
                                                     57.123
                                                             1.00 40.14
                                                                                   Ċ
     MOTA
           17247
                  CA
                      THR C 331
                                     27.719
                                             25.039
                                                             1.00 44.49
     MOTA
           17249
                  CB
                                                     57.137
     MOTA
           17251
                  OG1 THR C 331
                                     26.332
                                             25.263
                                                     56.874
                                                             1.00 47.97
                  CG2 THR C 331
30
                                             25.793
                                                             1.00 45.87
     MOTA
           17253
                                     28.457
                                                     56.054
                      THR C 331
                                  29.560 23.524
                                                     57.507
                                                             1.00 43.45
           17257
     MOTA
                  Ċ
                      THR C 331
                                     29.904
                                             23.749
                                                     58.675
                                                             1.00 41.19
     MOTA
           17258
                  0
                      VAL C 332
           17259
                                     30.416 23.306
                                                     56.515
                                                             1.00 39.96
     MOTA
                  N
                      VAL C 332
                                     31.828 23.320
                                                     56.680
                                                             1.00 35.05
     MOTA
           17261
                  CA
35
     ATOM
           17263
                  CB
                     VAL C 332
                                     32.397 21.988
                                                     56.442
                                                             1.00 34.40
                                   33.907 22.017
                                                             1.00 32.26
                  CG1 VAL C 332
                                                     56.732
     MOTA
           17265
                  CG2 VAL C 332
                                     31.704 21.009
           17269
                                                     57.307
                                                             1.00 35.49
     MOTA
                                                                                   С
     MOTA
           17273
                  С
                      VAL C 332
                                     32.330
                                             24.187
                                                     55.583
                                                             1.00 41.57
                                                                                   С
     ATOM
           17274
                  0
                      VAL C 332
                                     32.169
                                             23.850
                                                     54.413
                                                             1.00 41.46
                                                                                   0
40
     MOTA
           17275
                  N
                      MET C 333
                                     32.918
                                             25.314
                                                     55.956
                                                             1.00 43.32
                      MET C 333
     MOTA
           17277
                  CA
                                     33.419
                                             26.236
                                                     54.977
                                                             1.00 46.33
                      MET C 333
     ATOM
                                     33.426 27.663
           17279
                  CB
                                                     55.549
                                                             1.00 48.59
                      MET C 333
                                     32.239
                                             28.470
                                                             1.00 48.65
     ATOM
           17282
                                                     55.227
                                                                                   C
                  CG
     MOTA
           17285
                      MET C 333
                                     31.907 29.702
                                                     56.521
                                                             1.00 59.78
                  SD
45
                      MET C 333
                                     32.913 30.942
                                                     55.931
     ATOM
           17286
                  CE
                                                             1.00 59.17
     MOTA
           17290
                  С
                      MET C 333
                                     34.832 25.758
                                                     54.612
                                                             1.00 48.03
                      MET C 333
                                     35.809 26.193
     MOTA
           17291
                  0
                                                     55.201
                                                             1.00 42.88
     MOTA
           17292
                      GLY C 334
                                     34.915 24.862
                                                     53.635
                  N
                                                             1.00 48.50
                                                                                   N
                      GLY C 334
                                     36.160 24.240
     ATOM
           17294
                                                     53.247
                  CA
                                                             1.00 52.01
50
     ATOM
           17297
                      GLY C 334
                                     37.161
                                             25.091
                                                     52.503 1.00 53.89
                  C
                                                                                   C
                      GLY C 334
ALA C 335
     MOTA
           17298
                  0
                                     37.081
                                             26.315
                                                     52.511
                                                             1.00 58.04
                                                                                   0
                                             24.424
     MOTA
           17299
                  N
                                     38.112
                                                     51.850
                                                             1.00 51.10
                                                                                   N
     MOTA
           17301
                  CA
                      ALA C 335
                                     39.176 25.126
                                                     51.170
                                                             1.00 50.84
                                  40.226
                      ALA C 335
     MOTA
           17303
                  CB
                                             24.164
                                                     50.669
                                                             1.00 51.11
                      ALA C 335
55
                                     38.671
                                             25.963
                                                     50.024
     ATOM
           17307
                  C
                                                             1.00 53.88
                                                                                   C
                      ALA C 335
                                     39.280
                                             26.975
           17308
                                                     49.655
    ATOM
                  0
                                                             1.00 58.46
                                                                                   0
                      VAL C 336
           17309
                                     37.566
                                             25.592
                                                     49.424
     MOTA
                                                             1.00 52.66
                                                                                   N
                  N
     ATOM
           17311
                  CA
                      VAL C 336
                                     37.223
                                             26.366
                                                     48.255
                                                             1.00 56.89
    "ATOM
           17313
                  CB
                      VAL C 336
                                     36.226
                                            25.654
                                                     47.316
                                                             1.00 57.19
60
                  CG1 VAL C 336
                                     36.745
     ATOM
           17315
                                             24.245
                                                     46.966
                                                             1.00 56.50
                  CG2 VAL C 336
                                     34.848 25.609
           17319
                                                     47.913
     MOTA
                                                             1.00 59.09
```

| 5 | л ПОМ | 17323 | C | VAL C | 226 | • | 36.767 | 27.738 | 48.727 | 1.00 57.63 | | С |
|-----|-------|----------------|---------|-------|-----|---|------------------|------------------|------------------|--------------------------|----|--------|
| J | MOTA | | C | VAL C | | | 36.957 | 28.725 | 48.038 | 1.00 60.05 | | ŏ |
| | ATOM | 17324 | Ο. | ILE C | | | 36.198 | 27.799 | 49.915 | 1.00 53.26 | | N |
| | ATOM | 17325 17327 | N CA | ILE C | | | 35.714 | 29.050 | 50.421 | 1.00 54.88 | | Ċ |
| | ATOM | | | ILE C | | | 34.812 | 28.821 | 51.617 | 1.00 59.97 | | č |
| 10 | ATOM | 17329 | CB | | | | 33.605 | 28.021 | 51.167 | 1.00 53.37 | | Č |
| 10 | MOTA | 17331 | | ILE C | | | 33.536 | 27.873 | 49.654 | 1.00 65.75 | | c |
| | ATOM | 17334 | | | | | | 30.142 | 52.257 | 1.00 61.20 | | C |
| | ATOM | 17338 | | ILE C | | | 34.416 | 29.853 | 50.861 | 1.00 55.72 | | c |
| | ATOM | 17342 | C | ILE C | | | 36.884 | | 50.754 | 1.00 55.72 | | Ö |
| 15 | ATOM | 17343 | 0 | | | | 36.885 | 31.076 | 51.373 | 1.00 52.85 | | Ŋ |
| 15 | ATOM | 17344 | N | MET C | | , | 37.893 | 29.168 | | 1.00 32.83 | | C |
| | ATOM | 17346 | CA | MET C | | | 39.058 | 29.859 | 51.874 52.798 | 1.00 47.20 | ٠. | c |
| | MOTA | 17348 | CB | MET C | | | 39.791 39.048 | 28.921 28.822 | 54.095 | 1.00 47.20 | | c |
| _ | MOTA | 17351 | CG | | | | | | | 1.00 50.06 | | S |
| 20 | ATOM | 17354 | SD | MET C | | | 39.827 | 27.707 | 55.154 | 1.00 30.00 | | C |
| 20 | ATOM | 17355 | CE | MET C | | | 41.323 | 28.450 | 55.484 50.744 | 1.00 38.39 | | c |
| | MOTA | 17359 | C | MET C | | | 39.946 | 30.388 | | 1.00 42.32 | | 0 |
| | ATOM | 17360 | 0 | MET C | | | 40.483 | 31.476 | 50.842 | 1.00 47.16 | | N. |
| | ATOM | 17361 | N | GLU C | | | 40.093 | 29.619 | 49.685 | | | C |
| 25 | ATOM | 17363 | CA | GLU C | | • | 40.815 | 30.034 | 48.514 47.493 | 1.00 37.17 1.00 43.92 | | C |
| 25 | MOTA | 17365 | CB | GLU C | | | 40.806 | 28.877 | | 1.00 43.92 | | C |
| | ATOM | 17368 | CG | | | | 41.688 | 27.679 | 47.897 | 1.00 48.10 | | c |
| | ATOM | 17371 | CD | GLU C | | | 41.673 | 26.490 | 46.918 | 1.00 30.33 | | o |
| | ATOM | 17372 | | GLU C | | | 42.111 | 25.367 | 47.340 | 1.00 40.87 | | 0 |
| 20 | ATOM | 17373 | | GLU C | | | 41.232 | 26.671 31.374 | 45.751 | 1.00 41.22 | | C |
| 30 | ATOM | 17374 | C. | GLU C | | | 40.279 | | 47.900 | 1.00 39.02 | | 0 |
| | ATOM | 17375 | 0 | GLU C | | | 40.832 | 31.896 31.955 | 46.962 48.402 | 1.00 42.34 | | N |
| | ATOM | 17376 | N | GLY C | | | 39.213 | 33.297 | 47.960 | 1.00 33.46 | | C |
| | ATOM | 17378 | CA C | GLY C | | | 38.963 39.436 | 34.371 | 48.950 | 1.00 35.46 | | C. |
| 35 | MOTA | 17381 17382 | 0 | GLY C | | | 39.491 | 35.574 | 48.678 | 1.00 33.13 | | ŏ |
| رر | MOTA | 17383 | N | PHE C | | | 39.800 | 33.978 | 50.139 | 1.00 35.15 | | N |
| | ATOM | 17385 | CA | PHE C | | | 40.060 | 35.003 | 51.085 | 1.00 33.10 | | c |
| | ATOM | 17387 | CB | PHE C | | | 38.892 | 34.974 | 52.025 | 1.00 37.20 | | č |
| | ATOM | 17390 | CG | PHE C | | | 37.579 | 35.096 | 51.327 | 1.00 40.16 | | c |
| 40 | ATOM | 17391 | | PHE C | | | 36.751 | 33.993 | 51.165 | 1.00 41.87 | | č |
| 40 | ATOM | 17393 | | PHE C | | | 35.543 | 34.108 | 50.523 | 1.00 35.46 | | Ċ |
| | ATOM | 17395 | CZ | PHE C | | | 35.160 | 35.341 | 50.042 | 1.00 35.20 | | С |
| | ATOM | 17397 | | PHE C | | | 35.976 | 36.453 | 50.198 | 1.00 27.10 | • | C |
| | ATOM | 17399 | | PHE C | | | 37.160 | 36.331 | 50.830 | 1.00 37.05 | | С |
| 45 | ATOM | 17401 | C | PHE C | | | 41.393 | 34.881 | 51.842 | 1.00 37.72 | | С |
| | ATOM | 17402 | ō | PHE C | | | 42.042 | 33.895 | 51.736 | 1.00 35.29 | | 0 |
| | ATOM | 17403 | N | TYR C | | • | 41.793 | 35.948 | 52.531 | 1.00 38.91 | | N |
| | ATOM | 17405 | CA | TYR C | | | 42.864 | 35.934 | 53.519 | 1.00 40.66 | | С |
| | ATOM | 17407 | СВ | TYR C | | | 43.579 | 37.280 | 53.593 | 1.00 40.52 | | С |
| 50 | MOTA | 17410 | CG | TYR C | | • | 44.730 | 37.363 | 54.555 | 1.00 39.32 | | С |
| • | ATOM | 17411 | | TYR C | | | 45.634 | 36.362 | 54.621 | 1.00 37.44 | | С |
| | ATOM | 17413 | | TYR C | | | 46.694 | 36.415 | 55.487 | 1.00 39.89 | | С |
| | ATOM | 17415 | CZ | TYR C | | | 46.880 | 37.469 | 56.308 | 1.00 40.51 | | C |
| | ATOM | 17416 | ОН | TYR C | | | 48.015 | 37.396 | 57.146 | 1.00 35.08 | | 0 |
| 55 | ATOM | 17418 | | TYR C | | | 45.972 | 38.527 | 56.273 | 1.00 33.09 | • | С |
| 55 | ATOM | 17420 | | TYR C | | | 44.908 | 38.466 | 55.405 | 1.00 36.55 | | C |
| | ATOM | 17422 | C | TYR C | | | 41.948 | 35.832 | 54.690 | 1.00 39.22 | | Ċ, |
| | ATOM | 17423 | ō | TYR C | | | 41.035 | 36.677 | 54.718 | 1.00 33.31 | | o. |
| | ATOM | 17424 | N | VAL C | | | 42.160 | 34.836 | 55.588 | 1.00 31.59 | | N |
| 60 | ATOM | 17426 | CA | VAL C | | | 41.279 | 34.548 | 56.731 | 1.00 32.15 | | C |
| ~ 0 | MOTA | 17428 | СВ | VAL C | | | 40.744 | 33.094 | 56.729 | 1.00 34.63 | | C |
| | | | | | | | | | | 2.11 | | _ |

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C
                                         39.678
                                                           57.800
                                                                    1.00 37.79
     ATOM 17430
                   CG1 VAL C 343
                                                  32.894
                                                                    1.00 30.90
                   CG2 VAL C 343
                                         40.158
                                                  32.698
                                                           55.431
     MOTA
           17434
                                                                                            C
                                                                    1.00 34.71
                        VAL C 343
                                         42.126
                                                  34.646
                                                           57.971
     MOTA
           17438
                   С
                                                                                            0
                                                                    1.00 34.88
                        VAL C 343
                                         43.166
                                                  34.057
                                                           58.002
     MOTA
            17439
                   0
                        VAL C 344
                                                           58.991
                                                                    1.00 39.79
                                         41.668
                                                  35.362
     ATOM
            17440
                   N
                        VAL C 344
                                         42.422
                                                 35.621
                                                           60.206
                                                                    1.00 38.00
            17442
                   CA
10
     MOTA
                        VAL C 344
                                         42.381
                                                  37.141
                                                           60.498
                                                                    1.00 42.04
                                                                                            С
     MOTA
            17444
                   CB
                                                                                            С
                                                           61.904
                                                                    1.00 48.20
                   CG1 VAL C 344
                                         42.852
                                                  37.469
     MOTA
            17446
                                                                                            C
                                                                    1.00 39.85
                   CG2 VAL C 344
                                      43.247
                                                  37.919
                                                           59.538
     ATOM
            17450
                                                                    1.00 40.20
                                                                                            C
                        VAL C 344
                                         41.760
                                                  34.888
                                                           61.393
            17454
                   C
     MOTA
                                                                    1.00 39.35
                                                                                            0
                        VAL C 344
                                         40.616
                                                  35.179
                                                           61.718
           17455
15
     MOTA
                   0
                                                          62.045
                                                                    1.00 38.18
                                                                                            N
                                         42.440
                                                  33.940
     MOTA
           17456
                        PHE C 345
                   N
                                      41.849
42.267
41.608
40.459
39.861
                                                           63.219
                                                                    1.00 38.67
                                                                                            C
                                         41.849
                                                  33.277
           17458
                        PHE C 345
     MOTA
                   CA
                                                  31.811
                                                           63.250
                                                                    1.00 42.75
                                                                                            C
     ATOM
            17460
                    CB
                        PHE C 345
                                                           62.172 1.00 44.70
                                                                                            С
                                         41.608
                                                  30.985
     ATOM
           17463
                   CG
                       PHE C 345
                                                                    1.00 46.90
                                                                                            С
                                                           62.431
                    CD1 PHE C 345
                                                  30.278
20
     ATOM 17464
                                                  29.540
                                                                    1.00 45.20
                                                                                            С
                                         39.861
                                                           61.441
                   CE1 PHE C 345
     ATOM 17466
                                                           60.202
                                                                    1.00 37.04
                                                                                            C
                                      40.403
                                                  29.522
                   CZ
                        PHE C 345
     ATOM 17468
                                     41.5
42.133
42.193
                                                                                            C
                                                           59.941
                                                                    1.00 41.08
     ATOM 17470
                   CE2 PHE C 345
                                                  30.228
                                                           60.899
                                                                    1.00 40.32
                                                                                            C
                                                  30.944
                    CD2 PHE C 345
     ATOM 17472
                                     42.133 34.007 64.536

43.045 33.621 65.279

41.504 35.077 64.834

41.863 35.872 65.980

41.330 37.273 65.805

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                   OE2 GLU C 364
```

| 5 | 7 DOM | 17772 | С | GLU C 364 | 37 | 097 | 40.860 | 34.703 | 1.00 | 55.57 | | С |
|----|-------|-------|-----|-------------|------|----------------|--------|------------------|------|-------|----|-----|
| 3 | ATOM | | | GLU C 364 | | | 41.994 | 35.171 | 1.00 | 55.50 | | 0 |
| | ATOM | 17773 | | PHE C 365 | | 971 | 40.175 | 34.628 | 1.00 | | | N |
| | MOTA | 17774 | | | | 702 | 40.825 | 34.944 | 1.00 | | | С |
| - | MOTA | 17776 | | PHE C 365 | | 671 | 40.470 | 33.882 | | 48.33 | | С |
| | MOTA | 17778 | | PHE C 365 | | | 40.334 | 32.501 | | 48.95 | | C. |
| 10 | ATOM | 17781 | | PHE C 365 | | 219 | | 32.072 | | 49.95 | | С |
| | ATOM | 17782 | | PHE C 365 | | 692 | 39.123 | 30.789 | | 53.08 | | С |
| | MOTA | 17784 | | PHE C 365 | | 199 | 38.950 | 29.912 | | 55.82 | | Ċ |
| | ATOM | 17786 | | PHE C 365 | | 233 | 39.991 | | | 56.84 | | Ċ |
| | MOTA | 17788 | | PHE C 365 | | 750 | 41.271 | 30.319 | | 56.84 | | č |
| 15 | MOTA | 17790 | | PHE C 365 | | 243 | 41.424 | 31.616 | | 45.78 | ٠. | Ç. |
| | ATOM | 17792 | | PHE C 365 | | 054 | | 36.292 | | 49.51 | | o |
| | MOTA | 17793 | | PHE C 365 | | 976 | 40.993 | 36.576 | • | | | N |
| | ATOM | 17794 | | ARG C 366 | | 682 | 39.663 | 37.105 | | 45.57 | | C |
| • | ATOM | 17796 | | ARG C 366 | | 121 | 39.240 | 38.385 | | 41.73 | | Č |
| 20 | ATOM | 17798 | CB | ARG C 366 | | .243 | 38.013 | 38.194 | | 38.80 | | c |
| | MOTA | 17801 | CG | ARG C 366 | | .822 | 38.352 | 38.384 | | 37.22 | | |
| | ATOM | 17804 | CD | ARG C 366 | | . 802 | 37.311 | 38.128 | | 40.56 | | , C |
| • | MOTA | 17807 | NE | ARG C 366 | 31. | . 257 | 36.052 | 37.537 | | 48.25 | | N |
| | MOTA | 17809 | CZ | ARG C 366 | . 30 | . 432 | 35.033 | 37.321 | | 47.05 | | C |
| 25 | ATOM | 17810 | NH1 | ARG C 366 | 29 | .168 | 35.161 | 37.641 | | 44.28 | | N |
| | ATOM | 17813 | NH2 | ARG C 366 | 30 | .852 | 33.894 | 36.787 | _ | 53.80 | | N. |
| | ATOM | 17816 | Ċ | ARG C 366 | 35 | .212 | 38.904 | 39.367 | | 42.95 | | С |
| | MOTA | 17817 | 0 | ARG C 366 | 36 | .107 | 38.169 | 39.041 | | 47.17 | | 0 |
| | ATOM | 17818 | N | THR C 367 | 35 | .105 | 39.427 | 40.577 | | 45.66 | | N |
| 30 | ATOM | 17820 | CA | THR C 367 | 36 | .140 | 39.279 | 41.588 | | 47.80 | | С |
| 50 | ATOM | 17822 | СВ | THR C 367 | 36 | .868 | 40.622 | 41.749 | | 51.39 | | С |
| | ATOM | 17824 | | THR C 367 | 38 | .131 | 40.423 | 42.363 | | 57.38 | | 0 |
| | MOTA | 17826 | | THR C 367 | 36 | .156 | 41.538 | 42.774 | | 56.23 | | С |
| | ATOM | 17830 | C | THR C 367 | | .492 | 38.965 | 42.905 | 1.00 | 46.46 | | С |
| 35 | ATOM | 17831 | ō | THR C 367 | 34 | .522 | 39.642 | 43.277 | | 54.55 | | 0 |
| 33 | ATOM | 17832 | N | ALA C 368 | | .993 | 37.977 | 43.640 | 1.00 | 39.88 | | N |
| | ATOM | 17834 | CA | ALA C 368 | | .375 | 37.681 | 44.909 | | 32.52 | | С |
| | ATOM | 17836 | СВ | ALA C 368 | 36 | .048 | 36.619 | 45.526 | 1.00 | 37.31 | | С |
| | ATOM | 17840 | C | ALA C 368 | | .389 | 38.935 | 45.813 | 1.00 | 39.83 | | С |
| 40 | ATOM | 17841 | Ö | ALA C 368 | | .237 | 39.822 | 45.723 | 1.00 | 44.69 | | 0 |
| 40 | ATOM | 17842 | N | ALA C 369 | | .440 | 39.005 | 46.715 | 1.00 | 43.60 | | N |
| | ATOM | 17844 | CA | ALA C 369 | | .275 | 40.200 | 47.502 | 1.00 | 40.45 | | С |
| | ATOM | 17846 | СВ | ALA C 369 | | .188 | 40.996 | 46.899 | 1.00 | 43.87 | | С |
| | ATOM | 17850 | C | ALA C 369 | | .937 | 39.926 | 48.946 | 1.00 | 37.91 | | С |
| 45 | ATOM | 17851 | Ö | ALA C 369 | | .672 | 38.782 | 49.352 | 1.00 | 37.55 | • | 0 |
| 45 | ATOM | 17852 | N | VAL C 370 | | .960 | 41.017 | | 1.00 | 36.68 | | N |
| | | 17854 | CA | VAL C 370 | | .625 | 41.058 | 51.097 | 1.00 | 36.40 | | C |
| | MOTA | | CB | VAL C 370 | | | 40.835 | 51.938 | 1.00 | 34.82 | | С |
| | ATOM | 17856 | | VAL C 370 | | .375 | 40.751 | 53.345 | | 39.75 | | С |
| 50 | MOTA | 17858 | | VAL C 370 | | .455 | 39.559 | 51.558 | | 40.98 | | ·C |
| 50 | ATOM | 17862 | | | | 3.125 | 42.479 | 51.368 | | 38.45 | | С |
| | ATOM | 17866 | | VAL C 370 | | | 43.400 | | | 26.92 | | 0 |
| | MOTA | | | VAL C 370 | | 3.886 L.840 | 42.634 | 51.674 | | 44.21 | | N |
| | MOTA | | | GLU C 371 | | | 43.943 | 51.819 | | 47.61 | | C |
| | ATOM | | | GLU C 371 | | 1.246 | | 50.559 | | 51.18 | | Č |
| 55 | ATOM | | | GLU C 371 | | .441 | 44.204 | | | 54.46 | | Č |
| | MOTA | | | GLU C 371 | | 1.339 | 44.513 | 49.383 48.063 | | 57.83 | | c |
| | ATOM | | | GLU C 371 | | 714 | 44.152 | 47.072 | | 64.47 | | ő |
| | MOTA | | | GLU C 371 | | L.465 | | | | | | ő |
| | ATOM | | | 2 GLU C 371 | | 9.479 | | | | 63.16 | | c |
| 60 | MOTA | | | GLU C 371 | | 0.337 | | | | 48.24 | | o |
| | MOTA | 17882 | 0 | GLU C 371 | 2 | 9.893 | 43.081 | 33.3/6 | 1.00 | 47.20 | | |
| | | | | | | | | | | | | |

| 5 | MOTA | 17883 | N | GLY C | 372 | | 30.062 | 45.311 | 53,440 | | 50.29 | | | N |
|------------|------|-------|-----|--------|-----|---|--------|--------|--------|--------|-------|---|---|------------|
| • | ATOM | 17885 | CA | GLY C | 372 | | 29.156 | 45.560 | 54.560 | 1.00 | 50.67 | | • | С |
| | ATOM | 17888 | С | GLY C | 372 | | 29.149 | 47.025 | 54.947 | 1.00 | 50.50 | | | С |
| | ATOM | 17889 | 0 | GLY C | 372 | | 29.884 | 47.806 | 54.361 | 1.00 | 51.93 | | | 0 |
| • | ATOM | 17890 | N | PRO C | 373 | | 28.353 | 47.431 | 55.934 | 1.00 | 52.13 | | | N |
| 10 | ATOM | 17891 | CA | PRO C | | | 27.466 | 46.568 | 56.733 | 1.00 | 47.64 | | | С |
| 10 | ATOM | 17893 | СВ | PRO C | | | 27.318 | 47.351 | 58.016 | . 1.00 | 51.45 | | | С |
| | ATOM | 17896 | CG | PRO C | | | 27.992 | 48.699 | 57.790 | | 49.65 | | | С |
| | ATOM | 17899 | CD | PRO C | | | 28.278 | 48.839 | 56.356 | 1.00 | 47.50 | | | С |
| | ATOM | 17902 | C | PRO C | | | 26.077 | 46.434 | 56.223 | | 46.53 | | | С |
| 15 | ATOM | 17902 | Ö | PRO C | | | 25.632 | 47.293 | 55.527 | | 45.34 | | • | 0 |
| 15. | | 17903 | N | PHE C | | • | 25.398 | 45.365 | 56.607 | | 52.57 | , | | N |
| | MOTA | 17904 | CA | PHE C | | | 24.028 | 45.097 | 56.195 | | 50.90 | | | C |
| | ATOM | | | PHE C | | | 23.894 | 43.751 | 55.484 | | 49.66 | | | , C |
| | ATOM | 17908 | CB | PHE C | | | 24.437 | 43.797 | 54.115 | | 48.09 | | | C |
| 20 | ATOM | 17911 | CG | | | | 25.718 | 43.429 | 53.899 | | 39.08 | | | Ċ. |
| 20 | ATOM | 17912 | | PHE C | | • | 26.255 | 43.425 | 52.658 | | 42.90 | | | C |
| • | MOTA | 17914 | | PHE C | | | | 43.433 | 51.602 | | 42.40 | | | Č. |
| | ATOM | 17916 | CZ | PHE C | | | 25.507 | | | | 39.12 | • | | č |
| | MOTA | 17918 | | PHE C. | | | 24.192 | 44.339 | 51.799 | | 42.78 | | | C |
| | MOTA | 17920 | | PHE C | | | 23.660 | 44.272 | 53.042 | | | | | C |
| 25 | MOTA | 17922 | С | PHE C | | | 23.203 | 45.056 | 57.387 | | 52.02 | | | |
| | MOTA | 17923 | 0 | PHE C | | | 23.499 | 44.353 | 58.298 | | 54.34 | | | 0 |
| | MOTA | 17924 | N | VAL C | | | 22.141 | 45.825 | 57.369 | | 64.41 | | | N |
| | MOTA | 17926 | CA | VAL C | | | 21.259 | 45.867 | 58.496 | | 65.17 | | | C |
| | MOTA | 17928 | CB | VAL C | | | 20.319 | 47.035 | 58.465 | | 65.29 | | | C |
| 30 | MOTA | 17930 | CG1 | VAL C | 375 | | 18.943 | 46.570 | 58.832 | | 62.93 | | | C |
| , | ATOM | 17934 | CG2 | VAL C | 375 | | 20.850 | 48.116 | 59.416 | | 68.23 | | | С |
| | MOTA | 17938 | С | VAL C | 375 | | 20.504 | 44.604 | 58.423 | | 65.98 | | | C |
| • | ATOM | 17939 | 0 | VAL C | 375 | | 19.770 | 44.346 | 57.465 | | 61.21 | • | | О |
| | ATOM | 17940 | N . | THR C | 376 | | 20.735 | 43.830 | 59.472 | | 69.92 | | | N |
| 35 | MOTA | 17942 | CA | THR C | 376 | | 20.191 | 42.515 | 59.661 | | 72.22 | | | С |
| | ATOM | 17944 | CB | THR C | 376 | | 21.334 | 41.602 | 59.808 | 1.00 | 68.57 | | | C |
| | ATOM | 17946 | OG1 | THR C | 376 | | 22.053 | 41.618 | 58.582 | 1.00 | 71.14 | | | 0 |
| - | ATOM | 17948 | CG2 | THR C | 376 | | 20.874 | 40.181 | 59.945 | 1.00 | 74.54 | | | С |
| | ATOM | 17952 | С | THR C | 376 | | 19.394 | 42.475 | 60.931 | 1.00 | 76.89 | | | С |
| 40 | ATOM | 17953 | 0 | THR C | 376 | | 19.568 | 43.345 | 61.802 | 1.00 | 77.58 | • | | 0 |
| | ATOM | 17954 | N | LEU C | | | 18.515 | 41.483 | 61.041 | 1.00 | 78.66 | | | N |
| , . | ATOM | 17956 | CA | LEU C | 377 | | 17.779 | 41.340 | 62.271 | 1.00 | 81.96 | | | С |
| | ATOM | 17958 | СВ | LEU C | | | 16.384 | 42.007 | 62.166 | 1.00 | 82.78 | | | C |
| | ATOM | 17961 | CG | LEU C | | | 16.197 | 43.562 | 62.077 | 1.00 | 80.18 | | | С |
| 45 | ATOM | 17963 | | LEU C | | | 14.947 | 43.957 | 62.853 | | 78.29 | | | ·C |
| | MOTA | 17967 | | LEU C | | | 17.354 | 44.441 | 62.577 | 1.00 | 78.91 | | | С |
| | ATOM | 17971 | C | LEU C | | | 17.724 | 39.892 | 62.815 | 1.00 | 85.19 | | | С |
| | MOTA | 17972 | ŏ | LEU C | | | 17.679 | 38.869 | | 1.00 | 84.41 | | | 0 |
| | MOTA | 17973 | N | ASP C | | | 17.759 | 39.855 | 64.146 | | 85.34 | | | N |
| 50 | ATOM | 17975 | | ASP C | | | 17.597 | 38.638 | 64.925 | | 86.48 | | | Ċ |
| . 50 | | | | ASP C | | | 16.107 | 38.328 | 65.098 | | 87.44 | | | C |
| | MOTA | 17977 | CB | ASP C | | | 15.461 | 39.248 | 66.154 | | 89.47 | | | C |
| | ATOM | 17980 | | | | | 14.462 | | 65.855 | | 84.97 | | | Ö |
| | ATOM | 17981 | | ASP C | | | | | 67.324 | | 86.14 | | | ő |
| <i>c c</i> | ATOM | 17982 | | ASP C | | | 15.931 | 39.308 | | | | | | C. |
| 55 | ATOM | 17983 | С | ASP C | | | 18.427 | 37.522 | 64.336 | | 85.13 | | | |
| | ATOM | | 0 | ASP C | | | 17.942 | 36.486 | 63.887 | | 81.67 | | | 0 |
| | MOTA | 17985 | N | MET C | | | 19.722 | 37.805 | 64.374 | | 84.77 | | | N |
| | ATOM | 17987 | CA | MET C | | • | 20.750 | 36.965 | 63.819 | | 82.56 | | | C |
| | ATOM | 17989 | | MET C | | • | 22.027 | 37.805 | 63.684 | | 81.97 | | | С |
| 60 | ATOM | | | MET C | | | 21.955 | 38.836 | 62.581 | | 79.38 | | | С |
| | ATOM | 17995 | SÞ | MET C | 379 | | 23.553 | 39.475 | 62.065 | 1.00 | 83.45 | | • | S |

| _ | | | | · · · · · | 270 | 23.573 | 41.080 | 62.930 | 1.00 | 84.33 | | | С |
|------|--------|---------|------|-----------|------------|--------|--------|---------|------|----------|---|---|-----|
| 5 | ATOM | 17996. | | MET C | | 21.010 | 35.728 | 64.668 | | 84.75 | | | С |
| | MOTA | | | MET C | | 21.010 | 34.618 | 64.133 | | 82.43 | | | 0 . |
| | ATOM . | | 0 | MET C | | | | 65.986 | | 87.40 | | | N. |
| | ATOM | 18002 | N | GLU C | | 21.163 | 35.920 | 66.914 | | 87.60 | | | C |
| | MOTA | 18004 | CA | GLU C | | 21.555 | 34.840 | | | 89.46 | | | č |
| 10 | ATOM | 18006 | CB | GLU C | | 21.977 | 35.423 | 68.276 | | | | | c |
| | ATOM | 18009 | CG | GLU C | 380 | 22.952 | 34.592 | 69.137 | | 93.46 | | | c |
| | ATOM | | CD | GLU C | 380 | 23.920 | 33.680 | 68.372 | | 95.12 | | | |
| | ATOM | | | GLU C | | 25.124 | 34.033 | 68.271 | | 90.03 | | | 0 |
| | ATOM | | | GLU C | | 23.480 | 32.596 | 67.888 | | 96.29 | | | 0 . |
| 15 | ATOM | | C | GLU C | | 20.459 | 33.763 | 67.031 | | 86.12 | • | | C |
| 15 | | | Ö | GLU C | | | 32.687 | 67.584 | | 86.59 | | | 0 |
| | MOTA | | | ASP C | | 19.274 | 34.075 | 66.511 | | 83.49 | | | N |
| | MOTA | | | ASP C | 301 | | 33.064 | 66.258 | 1.00 | 81.88 | | | С |
| | ATOM | | CA | ASP C | | 16.884 | 33.717 | 66.074 | | 84.33 | | | С |
| | ATOM | | CB | | | 16.354 | 34.306 | | | 88.13 | | | С |
| 20 | ATOM - | | CG | ASP C | | 17.009 | 34.123 | 68.400 | | 92.81 | | | 0 |
| | MOTA | | ODI | ASP C | 381 | • | 34.957 | 67.412 | | 96.45 | | | 0 |
| | MOTA | | | ASP C | | 15.285 | | 65.026 | | 77.79 | | | С |
| | MOTA | 18027 | С | ASP C | | 18.542 | 32.177 | 64.663 | | 73.78 | | | 0 |
| | MOTA | 18028 | 0 | ASP C | | 17.711 | 31.347 | | | 76.40 | | | N |
| 25 | ATOM | 18029 | N | CYS C | 382 | 19.691 | 32.376 | 64.374 | | 74.85 | | | c · |
| | MOTA | 18031 | CA | CYS | | 20.187 | 31.458 | 63.331 | | 75.98 | | | č |
| | ATOM | 18033 | CB | | 382 | 20.891 | 32.215 | 62.222 | | | | | s |
| | ATOM | 18036 | SG | CYS C | 382 | 19.819 | 33.500 | 61.620 | | 81.03 | | | ,C |
| | MOTA | 18037 | С | CYS | 382 | 21.192 | 30.538 | 63.948 | 1.00 | 71.07 | | | Ö |
| 30 | ATOM | 18038 | 0 | CYS (| 382 | 21.755 | 29.673 | 63.284 | 1.00 | 71.77 | | * | |
| . 50 | ATOM | 18039 | N | | 383 | 21.432 | 30.753 | 65.230 | | 70.20 | | | N |
| | MOTA | 18041 | CA | | 383 | 22.315 | 29.896 | 65.987 | | 71.89 | | | C |
| | ATOM | 18044 | C | | C 383 | 21.508 | 28.693 | 66.386 | | 67.41 | | | C |
| ٠. | MOTA | 18045 | ō | | 383 | 20.307 | 28.772 | 66.344 | | 63.32 | | | 0 |
| 35 | | 18046 | N | | C 384 | 22.173 | 27.610 | 66.777 | | 70.66 | | | N |
| 33 | ATOM | 18048 | CA | | C 384 | 21.524 | 26.326 | 67.055 | | 70.77 | | | С |
| • | ATOM | 18050 | СВ | | C 384 | 22.069 | 25.337 | 66.056 | | 73.27 | | | C |
| | ATOM | 18053 | CG | | C 384 | 21.523 | 23.975 | 66.237 | | 78.48 | | | С |
| | | 18054 | | TYR | | 20.204 | 23.719 | 65.946 | | 81.09 | | | С |
| 40 | ATOM | | | TYR | | 19.676 | | 66.103 | 1.0 | 85.92 | | | С |
| 40 | ATOM | 18056 | CZ | | C 384 | 20.465 | | 66.560 | 1.0 | 86.01 | | | C |
| | ATOM | 18058 | OH | | C 384 | 19.876 | | 66.701 | 1.0 | 0 90.24 | | | 0 |
| | ATOM | 18059 | | | C 384 | 21.805 | | 66.865 | 1.0 | 0 85.31 | | | С |
| | MOTA | | CE | | C 384 | 22.322 | | | 1.0 | 0 81.62 | | | С |
| 40 | MOTA | | CD: | | | 21.815 | | | | 0 69.90 | | | С |
| 45 | ATOM | | C | | C 384 · | 22.877 | | | | 0 72.05 | | | 0 |
| | ATOM | | 0 | TIK | C 384 | 20.917 | | | | 0 70.22 | * | | N |
| | ATOM | | N | | C 385 | | | | | 0 71.13 | | | С |
| | ATOM | | CA | | C 385 | 21.075 | | | | 0 69.28 | | | С |
| | ATOM | 18071 | CB | ASN | C 385 | 20.189 | | | | 0 71.39 | | | С |
| 50 | ATOM | 18074 | CG | ASN | C 385 · | 20.760 | | | | 0 73.33 | | | O |
| | ATOM | 18075 | | | C 385 | 21.959 | | | | 0 59.22 | | | N |
| | ATOM | 18076 | ND | | C 385 | 19.922 | | | | | | _ | C |
| | ATOM | | C | ASN | C 385 | 20.886 | | | | 0 73.98 | | | Ô |
| | ATOM | | 0 | ASN | C 385 | 19.844 | | | | 0 78.23 | | | |
| 55 | ATOM | | OX | T ASN | C 385 | 21.764 | | | | 0 70.20 | | | 0 |
| | ATOM | | N | GLU | | 24.81 | | | | 0 49.83 | | | N |
| | ATOM | | CA | | | 24.832 | | | | 0 49.27 | | | C |
| | MOTA | | CB | | | 24.71 | 11.160 | | | 0 52.47 | | | С |
| | 1OTA | | CG | | | 24.17 | | | | 00 53.06 | | | C |
| 60 | | | CE | | | 23.83 | | 2 11.53 | | 0 54.58 | | | C |
| ου | 1OTA | | | 1 GLU | | 23.12 | | | | 00 58.12 | | | 0 |
| | MOTA | 1 18093 | O.E. | יד פדום | <i>J</i> 1 | | | | | | | | |

| | | | | | | | | | | , | | | |
|-------|--------------|-----------------|------------|------------|-------|----------|------------------|----------------|----------------|--------------------------|---|---|--------|
| 5 | MOTA | 18094 | OE2 | GLU I | 0 1 | | 24.276 | 12.444 | 10.373 | 1.00 51.77 | | | 0 |
| | ATOM | 18095 | С | GLU I | D 1 | | 26.172 | 9.309 | 14.292 | 1.00 53.40 | | | С |
| | MOTA | 18096 | 0 | GLU I | 0 1 | | 27.170 | 9.803 | 14.821 | 1.00 62.53 | | | 0 |
| | ATOM | 18099 | N . | VAL I | | | 26.219 | 8.207 | 13.540 | 1.00 50.49 | | | N |
| | ATOM . | 18101 | CA | VAL I | D 2 | | 27.451 | 7.883 | 12.839 | 1.00 47.46 | | | С |
| 10 | ATOM | 18103 | CB | VAL I | D · 2 | | 27.878 | 6.495 | 13.081 | 1.00 48.05 | | | С |
| | ATOM | 18105 | CG1 | VAL I | | | 28.636 | 6.435 | 14.387 | 1.00 43.66 | | | С |
| | MOTA | 18109 | CG2 | VAL I | D 2 | | 26.682 | 5,606 | 13.046 | 1.00 48.85 | | | С |
| .* | MOTA | 18113 | С | VAL I | | | 27.416 | 8.076 | 11.318 | 1.00 46.38 | | | C |
| | MOTA | 18114 | 0 | VAL I | | | 26.397 | 8.224 | 10.710 | 1.00 45.59 | | | 0 |
| .15 | MOTA | 18115 | N | ASN I | | • | 28.589 | 8.071 | 10.719 | 1.00 46.83 | | | N |
| • | MOTA | 18117 | CA | ASN I | | | 28.728 | 8.117 | 9.292 | 1.00 48.82 | | | Ç |
| - | MOTA | 18119 | CB | ASN I | | | 28.844 | 9.528 | 8.743 | 1.00 47.44 | | | С |
| ٠. | MOTA | 18122 | CG | ASN | | | 27.547 | 10.251 | 8.771 | 1.00 50.24 | | | C |
| | ATOM | 18123 | | ASN ! | | | 27.033 | 10.674 | 7.743 | 1.00 45.24 | | | 0 |
| 20 | MOTA | 18124 | | ASN I | | | 26.998 | 10.409 | 9.963 | 1.00 53.88 | | | N C |
| | MOTA | 18127 | С | ASN | | | 30.011 | 7.423 | 9.016 | 1.00 45.35 | • | | 0 |
| | MOTA | 18128 | | ASN | | | 30.876 | 8.042 | 8.462 | 1,00 .56.01 | | | 0 |
| | ATOM | 18129 | 0 | TOT 1 | | | 30.649 | 3.658 | 7.253 | 1.00 41.49 | | | C |
| | MOTA | 18130 | C . | LOL | | | 31.616 | 4.701 | 7.302 | 1.00 44.31 | | | C |
| 25 | MOTA | 18131 | CA | ror | | | 31.464 | 5.422 | 8.643 | 1.00 44.47 1.00 40.56 | | | N |
| | MOTA | 18132 | N | TOT | | | 30.059 | 5.809 | 8.714 9.742 | 1.00 40.30 | | | C |
| | ATOM | 18133 | CB | TOT | | | 31.620 | 4.400 | | 1.00 33.73 | | | c |
| | MOTA | 18134 | | LOL | | | 31.782 32.929 | 5.153 6.168 | 11.002 | 1.00 42.24 | | | c |
| 20. | MOTA | 18135 | | LOL | | | 32.012 | 4.153 | 12.156 | 1.00 30.05 | | | C |
| 30. | MOTA | 18136 | | LOL ALQ | | | 33.539 | 6.138 | 4.922 | 1.00 46.58 | | | ō |
| | MOTA | 18137 | 0 | ALQ | | | 32.895 | 5.448 | 4.118 | 1.00 40.59 | | • | Č |
| | ATOM | 18138. 18139 | C CA | ALQ | | | 31.531 | 4.899 | 4.429 | 1.00 34.48 | | | č |
| | ATOM | 18140 | CM | ALQ | | | 31.262 | 5.085 | 5.904 | 1.00 25.68 | | | Ċ |
| 35 | MOTA MOTA | 18141 | CB | ALQ | | | 30.525 | 5.761 | 3.689 | 1.00 32.81 | | | С |
| رږ | ATOM | 18142 | N | ALA | | | 33.833 | 4.377 | 4.106 | 1.00 47.34 | | | N |
| | ATOM | 18144 | CA | ALA | | | 35.183 | 4.871 | 3.785 | 1.00 46.63 | | | С |
| | ATOM | 18146 | CB | ALA | | | 35.992 | 3.752 | 3.209 | 1.00 48.42 | | | С |
| | ATOM | 18150 | С | ALA | | 5 | 35.139 | 6.050 | 2.825 | 1.00 48.53 | | | С |
| 40 | ATOM | 18151 | O | ALA | | 5 | 34.387 | 6.073 | 1.850 | 1.00 41.51 | | | 0 |
| | ATOM | 18154 | N | GLU | D 7 | 7 | 35.936 | 7.053 | 3.153 | 1.00 57.71 | | | N |
| | ATOM | 18156 | CA | GLU. | D 7 | 7 | 36.170 | 8.193 | 2.282 | 1.00 61.39 | | | C |
| | MOTA | 18158 | CB | GLU | D : | 7 | 37.103 | 9.150 | 2.997 | 1.00 63.36 | | | С |
| | MOTA | 18161 | CG | GLU | D 7 | 7 | 36.554 | 10.567 | 3.088 | 1.00 69.77 | | | С |
| 45 | MOTA | 18164 | CD | GLU | | 7 | 37.556 | 11.591 | 3.638 | 1.00 72.88 | | | С |
| | MOTA | 18165 | OE1 | GLU | D i | 7 | 37.130 | 12.437 | 4.470 | 1.00 71.19 | | | 0 |
| | ATOM | 18166 | OE2 | GLU | | 7 | 38.753 | 11.548 | 3.245 | 1.00 71.30 | | | 0 |
| | ATOM | 18167 | С | GLU | | 7 | 36.746 | 7.878 | 0.873 | | | | С |
| | MOTA | 18168 | 0 | GLU | | 7 | 36.460 | 8.610 | -0.067 | 1.00 59.17 | | | 0 |
| 50 | ATOM | 18169 | N | PHE | | В | 37.554 | 6.833 | 0.708 | 1.00 64.51 | | | N |
| | ATOM | 18171 | CA | PHE | | 3 | 38.046 | 6.472 | -0.636 | 1.00 66.42 | | | C |
| | MOTA | 18173 | CB | PHE | | 8 | 37.450 | 5.145 | -1.093 | 1.00 61.61 | • | | C |
| | ATOM | 18176 | CG | PHE | | 8 | 38.061 | 4.586 | -2.379 | 1.00 58.86 | • | | C |
| . سرم | ATOM | 18177 | | PHE | | 8 | 37.441 | 4.769 | -3.602 | 1.00 59.33 | | | C |
| 55 | ATOM | 18179 | | PHE | | 8 | 37.986 | 4.253 | -4.767 | 1.00 58.96 | | - | C |
| | MOTA | 18181 | CZ | PHE | | В | 39.174 | 3.536 | -4.731 | 1.00 60.39 | | | C |
| | ATOM | 18183 | | PHE | | 8 | 39.800 | 3.345 | -3.536 | 1.00 58.60 | | | C |
| | ATOM | 18185 | | PHE | | B · | 39.239 | 3.869 | -2.355 | 1.00 59.06 | | | C |
| 60 | ATOM | 18187 | C | PHE | | 8 o · | 37.706 | 7.526 | -1.692 | 1.00 70.25 | | • | 0 |
| 60 | ATOM | 18188 | 0 | PHE | | В . | 36.951 | 7.302 | -2.641 | 1.00 73.78 | | • | |
| | MOTA | 18189 | OXT | PHE | ט | 8 | 38.159 | 8.667 | -1.670 | 1.00 76.04 | | | 0 |

| 5 | ATOM | 18190 | N. | GLU | E | 1 | | 3.521 | 56.829 | 27.990 | 1.00 51.90 | | | N |
|----|--------------|-------|----------|------------|----|-----|---|--------|--------|--------|------------|----|---|-----|
| | ATOM | 18192 | CA | GLU : | E | 1 | | 4.813 | 56.347 | 27.405 | 1.00 53.95 | | | C. |
| | MOTA | 18194 | CB | GLU | É | 1 | | 4.748 | 54.908 | 26.863 | 1.00 52.89 | | | С |
| | MOTA | 18197 | CG · | GLU : | E | 1 | | 6.020 | 54.441 | 26.144 | 1.00 54.53 | | | С |
| | MOTA | 18200 | CD | GLU | E | 1 | | 5.940 | 53.023 | 25.544 | 1.00 61.12 | | | С |
| 10 | ATOM | 18201 | OE1 | GLU | E | 1 | | 4.802 | 52.481 | 25.400 | 1.00 68.56 | | | 0 |
| | MOTA | 18202 | OE2 | GLU | E | 1 | | 7.009 | 52.427 | 25.193 | 1.00 55.04 | | | O. |
| | ATOM | 18203 | С | GLU | E. | 1 | | 5.206 | 57.280 | 26.290 | 1.00 56.24 | | | С |
| | ATOM | 18204 | 0 | GLU | E | 1 | | 4.726 | 57.179 | 25.177 | 1.00 58.77 | | | 0 |
| - | ATOM | 18207 | N | VAL | E | 2 | | 6.069 | 58.225 | 26.625 | 1.00 60.38 | | | N |
| 15 | ATOM | 18209 | CA | VAL | Ε. | 2 | | 6.748 | 59.058 | 25.641 | 1.00 55.03 | | | C · |
| | ATOM | 18211 | СВ | VAL | E | 2 | | 7.513 | 60.074 | 26.359 | 1.00 53.73 | | | С |
| • | ATOM | 18213 | | VAL | E | 2 | | 6.581 | 60.848 | 27.263 | 1.00 55.96 | | • | С |
| | ATOM | 18217 | | VAL | | 2 | | 8.615 | 59.394 | 27.171 | 1.00 56.70 | | | С |
| • | ATOM | 18221 | C | VAL | | 2 | | 7.758 | 58.285 | 24.804 | 1.00 54.06 | | | С |
| 20 | ATOM | 18222 | 0. | VAL | | 2 | | 8.268 | 57.267 | 25.214 | 1.00 51.79 | | | 0 |
| 20 | ATOM | 18223 | N | ASN | | 3 | | 8.053 | 58.785 | 23.618 | 1.00 51.49 | | | N |
| | ATOM | 18225 | CA | ASN | | 3 | | 9.062 | 58.167 | 22.787 | 1.00 49.08 | | | С |
| | ATOM | 18227 | СВ | ASN | | 3 | | 8.502 | 56.972 | 22.011 | 1.00 52.23 | • | | С |
| | ATOM | 18230 | CG | ASN | | 3 | | 8.790 | 55.632 | 22.678 | 1.00 58.18 | • | | С |
| 25 | ATOM | 18231 | | ASN | | 3 | | 9.955 | 55.264 | 22.882 | 1.00 65.86 | | | 0 |
| LJ | ATOM | 18232 | | ASN | | 3 | | 7.724 | 54.885 | 23.009 | 1.00 59.14 | | | N |
| | ATOM | 18235 | Ç | ASN | | 3 | | 9.599 | 59.235 | 21.836 | 1.00 48.29 | | | С |
| | ATOM | 18236 | Ö | ASN | | 3 | | 9.547 | 59.112 | 20.605 | 1.00 43.64 | | | 0 |
| | ATOM | 18237 | Ö | LOL | | 4 | | 12.598 | 62.494 | 21.688 | 1.00 44.76 | | | 0 |
| 30 | ATOM | 18238 | c | FOF | | 4 | | 11.793 | 61.498 | 21.082 | 1.00 36.75 | | | С |
| 30 | ATOM | 18239 | CA | LOL | | 4 | | 10.394 | 61.683 | 21.640 | 1.00 39.29 | | | С |
| | MOTA | 18240 | N | FOF | | 4 | | 10.081 | 60.567 | 22.545 | 1.00 35.78 | ٠. | • | N |
| | ATOM | 18241 | СВ | TOT | | 4 | | 10.243 | 62.899 | 22.530 | 1.00 30.76 | | | С |
| | ATOM | 18242 | CG | LOL | | 4 | | 8.730 | 62.693 | 22.652 | 1.00 40.35 | | | C |
| 35 | ATOM | 18243 | | LOL | | 4 | | 8.185 | 62.234 | 21.296 | 1.00 31.81 | | | С |
| 33 | ATOM | 18244 | | POP | | 4 | | 8.003 | 63.914 | 23.151 | 1.00 38.31 | | | С |
| | ATOM | 18245 | 0 | ALQ | | 5 | | 12.574 | 60.630 | 18.017 | 1.00 56.62 | | | 0 |
| | ATOM | 18246 | Ċ | ALQ | | 5 | | 12.792 | 61.258 | 19.046 | 1.00 45.00 | | | С |
| | ATOM | 18247 | CA | ALQ | | 5 | | 13.506 | 60.509 | 20.107 | 1.00 39.17 | | | С |
| 40 | ATOM | 18248 | CM | ALQ | | 5 | | 12.383 | 59.943 | 20.954 | 1.00 33.18 | | | С |
| 40 | ATOM | 18249 | СВ | ALQ | | 5 | | 14.198 | 59.370 | 19.382 | 1.00 38.30 | | | С |
| | ATOM | 18250 | N | ALA | | 6 | | 13.763 | 61.587 | 17.911 | 1.00 53.06 | | | N |
| | ATOM | 18252 | CA | ALA | | 6 | | 13.416 | 62.316 | 16.681 | 1.00 48.77 | | | С |
| | ATOM | 18254 | CB | ALA | | 6 | • | 14.238 | 63.578 | 16.590 | 1.00 46.81 | | | С |
| 45 | ATOM | 18258 | C | ALA | | 6 | | 13.739 | 61.376 | 15.550 | 1.00 56.62 | | | С |
| 73 | ATOM | 18259 | ŏ | ALA | | 6 | | 14.884 | 61.001 | 15.355 | 1.00 60.60 | | | 0 |
| | ATOM | 18262 | N . | GLU | | 7 | • | 12.718 | 60.941 | 14.836 | 1.00 66.83 | | | N |
| | ATOM | 18264 | CA | GLU | | 7 | | 12.894 | 60.209 | 13.578 | 1.00 70.79 | | | С |
| - | MOTA | 18266 | CB | GLU | | 7 | | 11.658 | 60.366 | 12.670 | 1.00 71.58 | | | C |
| 50 | | 18269 | CG | GLU | | . 7 | | 11.195 | 58.999 | 12.147 | 1.00 74.78 | | | С |
| 30 | ATOM ATOM | 18272 | CD | GLU | | 7 | | 9.767 | 58.949 | 11.583 | 1.00 77.65 | ٠. | | С |
| | | 18273 | | GLU | | 7. | | 9.502 | 59.494 | 10.475 | 1.00 71.21 | | | 0 |
| | MOTA | 18274 | | GLU | | 7 | | 8.907 | 58.325 | 12.252 | 1.00 77.08 | | | 0 |
| | ATOM | 18275 | C | GLU | | 7 | | 14.184 | 60.468 | 12.764 | 1.00 72.67 | | | С |
| 55 | ATOM | | | GLU | | 7 | | 15.094 | 59.622 | 12.765 | 1.00 77.73 | | | O |
| 55 | ATOM | 18276 | O N | | | 8 | | 14.297 | 61.598 | 12.705 | 1.00 75.16 | | | N |
| | ATOM | 18277 | N | PHE PHE | | 8 | | 15.396 | 61.740 | 11.113 | 1.00 80.96 | | | C |
| | MOTA | 18279 | CA CB | | | 8 | | 16.737 | 61.952 | 11.801 | 1.00 82.87 | | | C. |
| • | ATOM | 18281 | | | | 8 | | 17.803 | 62.573 | | 1.00 82.87 | | | c |
| 60 | MOTA | 18284 | CG | PHE | | 8 | | 18.769 | 61.793 | | 1.00 83.54 | | | č |
| 60 | MOTA | 18285 | | PHE | | | | 19.751 | 62.381 | | 1.00 81.99 | | | c |
| | MOTA | 18287 | CEI | PHE | E. | 8 | | 19.191 | 02.301 | 2.473 | 1.00 01.99 | | | _ |

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MOTA
           18289
                  CZ
                       PHE E
                               8
                                       19.763 63.746
                                                        9.316 1.00 83.35
     MOTA
            18291
                   CE2 PHE E
                               8
                                       18.811
                                               64.520
                                                        9.944
                                                               1.00 82.55
     MOTA
           18293
                   CD2 PHE E
                               8
                                       17.841
                                               63.934
                                                       10.739
                                                               1.00 82.70
     MOTA
           18295
                   С
                       PHE E
                               8
                                       15.507
                                               60.437
                                                       10.291
                                                               1.00 85.47
     ATOM
           18296
                   0
                       PHE E
                               8
                                       16.608
                                               59.978
                                                        9.946
                                                               1.00 83.09
                                                                                     0
                              . 8
10
     MOTA
           18297
                   OXT PHE E
                                    14.521
                                               59.767
                                                        9.937
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           18298
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                                                       47.515
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                  CA
                       GLU F
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                                                       48.535
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                       GLU F
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                                                       48.449
                                                               1.00 55.81
           18305
     MOTA
                   CG
                       GLU F
                               1
                                      36.898
                                              15.591
                                                       48.922
                                                               1.00 53.48
15
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                       GLU F
                               1
                                      35.432
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                                                               1.00 57.95
                                    35.172
     ATOM
           18309
                   OE1 GLU F
                               1
                                              14.718
                                                       47.492
                                                               1.00 57.16
     ATOM
           18310
                  OE2 GLU F
                             . 1
                                      34.540
                                              15.499
                                                       49.515
                                                               1.00 46.53
                                                                                     0
     ATOM
           18311
                  С
                       GLU F
                               1
                                      39.838
                                              14.584
                                                       49.925
                                                               1.00 56.46
                                                                                     C
     ATOM
           18312
                       GLU F
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                  .0
                               1
                                                       50.262
                                                               1.00 59.04
20
     MOTA
           18315
                       VAL F
                  N
                               2
                                      40.171 . 15.626
                                                       50.694
                                                              1.00 52.85
                                                                                     N
     ATOM
           18317
                  CA
                       VAL F
                               2
                                      40.258 15.529
                                                       52.154
                                                               1.00 48.66
                                                                                     C
    . ATOM
           18319
                  CB
                       VAL F
                               2
                                      41.331 16.368
                                                       52.682
                                                               1.00 45.45
                                                                                     C
     MOTA
           18321
                  CG1 VAL F
                               2
                                      42.586 15.583
                                                       52.593
                                                               1.00 48.71
                                                                                     C
     ATOM
           18325
                  CG2 VAL F
                               2
                                      41.395 17.658
                                                       51.885
                                                               1.00 48.21
                                                                                     C
25
     MOTA
           18329
                  С
                       VAL F
                               2
                                      39.011 15.976
                                                       52.885
                                                               1.00 45.82
                                                                                     C
     MOTA
           18330
                  0
                       VAL F
                               2
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                                              16.826
                                                       52.430
                                                               1.00 52.38
                                                                                     0
     ATOM
           18331
                       ASN F
                  N
                               3
                                      38.762
                                              15.399
                                                       54.047
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                                                                                   N
     MOTA
           18333
                      ASN F
                  CA
                               3
                                      37.566
                                              15.702
                                                       54.814
                                                               1.00 48.46
                                                                                     C
     MOTA
           18335
                      ASN F
                  CB
                               3
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                                              14.705
                                                       54.512
                                                               1.00 46.45
                                                                                     С
30
     ATOM
           18338
                                      35.499
                  CG
                      ASN F
                               3
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                                                       53.371
                                                               1.00 48.95
     ATOM
           18339
                  OD1 ASN F
                               3
                                      34.662 16.042
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                                                               1.00 56.94
     ATOM
           18340
                  ND2 ASN F
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                                                       52.147
                                                               1.00 41.31
                                                                                     N
     ATOM
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                  С
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                                                               1.00 48.81
                                                                                     С
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                                                       56.945
                                                               1.00 46.42
                                                                                     0
35
                      LOL F
    · ATOM
           18345
                  0
                                    39.109 18.145
                               4
                                                       59.529
                                                               1.00 30.33
                                                                                     0
     ATOM
           18346
                  С
                      LOL F
                               4
                                      39.139 16.727
                                                       59.642
                                                               1.00 37.57
                                                                                     C
     ATOM
           18347
                  CA
                      LOL F
                               4
                                      39.449
                                              15.978
                                                       58.340
                                                               1.00 34.22
     ATOM
           18348
                  N
                       LOL F
                               4
                                      38.607
                                              16.653
                                                       57.414
                                                               1.00 33.81
     MOTA
           18349
                  CB
                      LOL F
                               4
                                      40.854
                                              16.178
                                                       57.816
                                                               1.00 29.74
                                                                                     С
40
     ATOM
           18350
                      LOL F
                  CG
                               4
                                      41.230
                                              14.854
                                                       57.136
                                                               1.00 42.88
                                                                                     С
     ATOM
           18351
                  CD2 LOL F
                                      40.898 13.685
                             . 4
                                                       58.067
                                                               1.00 44.40
                                                                                     C
     ATOM
           18352
                  CD1 LOL F
                                     42.690 14.689
                               4
                                                       56.716
                                                               1.00 33.62
                                                                                     С
     ATOM
           18353
                  0
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                               5
                                      37.076 16.340
                                                       61.729
                                                               1.00 51.12
                                                                                     0
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           18354
                  C
                      ALQ F
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                                      37.482 17.448
                                                       61.387
                                                               1.00 44.19
                                                                                     C
45
     ATOM
           18355
                  CA
                      ALQ F
                               5
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                                                       60.039
                                                               1.00 45.38
                                                                                     С
     ATOM
           18356
                  CM
                      ALQ F
                               5
                                      37.387 16.833
                                                       58.971
                                                               1.00 30.19
                                                                                     С
     ATOM
           18357
                      ALQ F
                  CB
                               5
                                      35.522 17.952
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                                                       60.244
                                                               1.00 38.38
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           18358
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50
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                                                                                     C
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           18366
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                      ALA F
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                               6
                                                       63.915
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                                                                                     C
    MOTA
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                                                       64.126
                                                               1.00 60.39
                                                                                     0
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           18370
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                                              14.325
                                                       63.591
                                                               1.00 61.57
                                                                                     N
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           18372
                      GLU F
                               7
                  CA
                                      34.181 13.687
                                                       63.917
                                                               1.00 67.60
                                                                                     C
55
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           18374
                      GLU F
                  CB
                               7
                                     34.182
                                              12.237
                                                       63.388
                                                               1.00 70.70
                                                                                     C
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           18377
                  CG
                      GLU F
                               7
                                      32.813
                                              11.775
                                                       62.910
                                                               1.00 73.43
                                                                                     C
     ATOM
           18380
                      GLU F
                  CD
                               7
                                     -32.354
                                              10.447
                                                       63.500
                                                               1.00 77.46
                                                                                     C
     .ATOM
           18381
                  OE1 GLU F
                               7
                                      32.607
                                              10.173
                                                       64.697
                                                               1.00 77.46
     ATOM
           18382
                  OE2 GLU F
                               7
                                      31.714
                                               9.677
                                                       62.756
                                                               1.00 78.85
60
     ATOM
           18383
                      GLU F
                  C
                               7
                                      33.791
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                                                       65.424
                                                               1.00 65,86
     ATOM
           18384
                      GLU F
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                               7
                                      33.074
                                              12.629
                                                       65.731
                                                               1.00 68.96
```

| ,5 | ATOM · | 18385 | N | PHE | F | 8 | | 34.287 | 14.366 | 66.347 | 1.00 | 67.95 | | N |
|-------------|--------|-------|-----|-----|----|----|---|----------|---------|---------|------|--------|-----|-----|
| ,0 | ATOM | 18387 | CA | PHE | | 8 | | 33.718 | 14.541 | 67.716 | | 67.25 | | С |
| | ATOM | 18389 | CB | PHE | | 8 | | 34.303 | 15.837 | 68.301 | 1.00 | 68.83 | | ·C |
| | ATOM | 18392 | CG | PHE | | 8 | | 33.612 | 16.393 | 69.544 | | 64.14 | • | С |
| | ATOM | 18393 | | PHE | | 8 | | 32.493 | 17.192 | 69.441 | | 65.62 | | С |
| 10 | ATOM | 18395 | | PHE | | 8 | | 31.873 | 17.724 | 70.583 | | 64.20 | | Č |
| 10 | ATOM | 18397 | CZ | PHE | | 8 | | 32.376 | 17.472 | 71.840 | | 63.31 | | Č |
| | | | | PHE | | 8 | | 33.496 | 16.688 | 71.971 | | 65.43 | | č |
| | ATOM | 18399 | | | | | | 34.123 | 16.150 | 70.817 | | 66.04 | | Č |
| | ATOM | 18401 | | PHE | | 8 | | | | 67.761 | | 71.68 | • | č |
| 1.0 | ATOM | 18403 | C | PHE | | 8 | | 32.209 | 14.659 | 68.854 | | 73.64 | | Ö |
| 15 | ATOM | 18404 | 0 | PHE | | 8 | | 31.610 | 14.612 | | | 76.55 | | Ö |
| | ATOM | 18405 | | PHE | | 8 | | 31.569 | 14.808 | 66.717 | | | | 0 |
| | ATOM | 18406 | 0 | НОН | | 1 | | 39.700 | 13.653 | 43.690 | | | | |
| | ATOM | 18409 | 0 | НОН | | 2 | | 17.999 | -0.835 | 18.526 | | 57.08 | | 0 |
| / | MOTA | 18412 | 0 | нон | | 3 | | -2.213 | 39.679 | 44.264 | | 47.81. | | 0 |
| 20 | ATOM | 18415 | 0 | HOH | | 4 | | 44.390 | 21.700 | 54.614 | | 36.23 | • | 0 |
| | ATOM | 18418 | 0 | HOH | | 5 | | 44.036 | 10.520 | 13.671 | | 20.25 | | 0 |
| | MOTA | 18421 | 0 | HOH | W | 6 | | 21.081 | | 18.984 | | 79.68 | | 0 |
| | MOTA | 18424 | 0 | нон | W | 7 | | 12.954 | 48.886 | | | 47.92 | | 0 |
| • | ATOM | 18427 | 0 | HOH | W | 8 | | 8.570 | 89.322 | 9.495 | | 42.50 | | O |
| 25 | ATOM | 18430 | 0 | HOH | W | 9 | | 25.965 | -8.446 | -10.244 | 1.00 | 58.04 | | 0 |
| | MOTA | 18433 | σ | нон | W | 10 | | 11.743 | 63.828 | 30.252 | 1.00 | 60.50 | | 0 |
| | ATOM | 18436 | o | НОН | W | 11 | | -0.897 | 57.335 | 42.929 | 1.00 | 57.91 | | Ó |
| | ATOM | 18439 | 0 | НОН | | 12 | | 52.750 | 29.899 | 42.854 | 1.00 | 71.96 | | 0 |
| | MOTA | 18442 | 0 | нон | | 13 | | 31.267 | 56.125 | 22.788 | 1.00 | 67.37 | | О |
| 30 | ATOM | 18445 | o | нон | | 14 | | -0.501 | 17.272 | 5.350 | 1.00 | 49.57 | | 0 |
| 20 | ATOM | 18448 | Ō | НОН | | 15 | | 19.139 | 31.098 | 19.928 | | 53.73 | • | 0 |
| | ATOM | 18451 | ō | нон | | 16 | | 29.653 | 40.187 | 36.475 | 1.00 | 51.39 | • | 0 - |
| | ATOM | 18454 | ō | НОН | | 17 | | 1.702 | 54.764 | | | 59.48 | * | 0 |
| | ATOM | 18457 | Ō | нон | | 18 | | | -19.576 | 2.357 | | 54.90 | | 0 |
| 35 | ATOM | 18460 | Ö | нон | | 19 | • | 10.345 | 16.962 | 33.276 | | 66.13 | | 0 |
| 33 | ATOM | 18463 | ő | НОН | | 20 | | 9.735 | 17.583 | -5.490 | | 62.55 | | 0 |
| | ATOM | 18466 | Ö | нон | | 21 | | 16.189 | 57.395 | 15.723 | | 60.50 | | O |
| | ATOM | 18469 | ó | нон | | 22 | | | | 18.933 | | 43.39 | | Ō |
| | MOTA | 18472 | Ö | нон | | 23 | | 26.061 | -0.244 | 12.926 | | 35.89 | | 0 |
| 40 | MOTA | 18475 | o | НОН | | 24 | | 21.349 | | -14.919 | | 60.98 | | ō |
| 40 | | | | НОН | | 25 | | -4.354 | | 53.329 | | 77.11 | | Ö |
| | MOTA | 18478 | 0 | | | 26 | | 46.391 | 31.873 | 42.449 | | 46.27 | | ŏ |
| | ATOM | 18481 | 0 | HOH | | | | 5.794 | | 30.466 | | 56.03 | | Ö |
| | ATOM | 18484 | 0 | HOH | | 27 | | | 14.925 | | | | | ő |
| A.E. | ATOM | 18487 | 0 | НОН | | 28 | | 18.066 | 33.687 | 53.506 | | 60.88 | | Ö |
| .45 | ATOM | 18490 | 0 | нон | | 29 | | 34.788 | 61.731 | 39,462 | | 47.79 | | O' |
| | MOTA | 18493 | 0 | HOH | | 30 | | 21.025 | 22.947 | 1.341 | | 59.51 | | |
| | ATOM | 18496 | 0 | НОН | | 31 | • | 16.949 | 23.886 | 38.354 | | 45.81 | | 0 |
| | MOTA | 18499 | 0 | НОН | | 32 | | 39.142 | 5.166 | 3.509 | | 66.57 | | 0 |
| | ATOM | 18502 | 0 | HOH | | 33 | | 60.666 | 20.142 | 53.793 | | 44.92 | . , | 0 |
| 50 . | ATOM | 18505 | ·O | HOH | | 34 | | . 42.265 | 8.229 | -0.588 | | 60.46 | | 0 |
| | ATOM | 18508 | 0 | HOH | | 35 | | 32.860 | 14.034 | 60.875 | | 60.98 | | 0 |
| | ATOM | 18511 | 0 | нон | W | 36 | | 32.941 | 17.022 | 57.493 | | 38.19 | | 0 |
| | ATOM | 18514 | Ο. | HOH | W | 37 | | 29.695 | 61.886 | 47.641 | | 59.00 | | 0 |
| | ATOM | 18517 | 0 | HOH | W | 38 | | 33.674 | -12.279 | -2.746 | 1.00 | 45.53 | | 0 |
| 55 | MOTA | 18520 | 0 | нон | W | 39 | | 41.413 | -14.843 | 19.171 | 1.00 | 65.48 | | 0 |
| | ATOM | 18523 | 0 | нон | | 40 | | 24.064 | | -21.588 | | 70.17 | | 0 |
| | ATOM | 18526 | 0 | нон | | 41 | | 23.715 | 82.758 | 18.726 | 1.00 | 35.41 | | 0 |
| | ATOM | 18529 | ō | нон | | 42 | | | -13.020 | | | 52.35 | | 0 |
| | ATOM | 18532 | Ŏ | нон | | 43 | | | -15.675 | -0.741 | | 53.72 | • | 0 |
| 60 | ATOM | 18535 | Ö | нон | | 44 | | 27.524 | 78.411 | | | 48.20 | | 0 |
| - - | ATOM | 18538 | | НОН | | 45 | | 31.107 | 72.075 | | | 47.99 | | 0 |
| | 011 | 10000 | . – | | •• | | | - 1 | | | | | | |

| | | <u>.</u> | | | | | | _ | | | | |
|------------|--------------|----------------|-----|---------|----------|-------------------------|-----------------------|------------------|---------|--------------------|---|----|
| -5 | ATOM | 18541 | 0 | нон м | 46 | 21.564 34 | 1.567 3 | 37.693 | 1.00 | 46.25 | | 0 |
| | ATOM | 18544 | 0 | HOH W | 47 | 21.067 71 | 1.763 2 | 21.267 | 1.00 | 39.24 | | o |
| | MOTA | 18547 | О | HOH W | | 10.404 9 | 0.098 2 | 24.542 | 1.00 | 57.88 | | 0 |
| | ATOM | 18550 | 0 | HOH W | | | .013 3 | 32.485 | 1.00 | 60.14 | | 0 |
| 10 | ATOM | 18553 | 0 | HOH W | | | | 18.467 | 1.00 | | | 0 |
| 10 | ATOM | 18556 | 0 | HOH W | | | | 17.061 | 1.00 | 42 _. 07 | • | 0 |
| | ATOM | 18559 | 0 | HOH W | | | | 39.473 | 1.00 | | | 0 |
| | ATOM | 18562 | 0 | HOH W | | 55.509 -10 | | 15.668 | 1.00 | | • | 0 |
| | ATOM | 18565 | 0 | HOH W | | | | 24.706 | 1.00 | | | 0 |
| 15 | ATOM ATOM | 18568 18571 | 0 | HOH W | | | | 51.342 | 1.00 | | | 0 |
| 15 | ATOM | 18574 | 0 | W HOH W | | | and the second second | 24.624 | 1.00 | | | 0, |
| | ATOM | 18577 | o | HOH W | | | | 13.632 39.068 | 1.00 | | | 0 |
| | ATOM | 18580 | Ö | HOH W | | 27.493 -10 | | 19.656 | 1.00 8 | | | 0 |
| • | ATOM | 18583 | Ö | HOH W | | | | 15.173 | 1.00 | | | 0 |
| 20 | ATOM | 18586 | ō. | HOH W | | | | 39.341 | 1.00 8 | | | 0 |
| | ATOM | 18589 | 0 | HOH W | | | | 7.199 | 1.00 | | | o |
| | MOTA, | 18592 | 0 | HOH W | | | | 7.209 | 1.00 | | | o |
| | MOTA | 18595 | 0 | HOH W | | | | 8.144 | 1.00 | | | Ö |
| | ATOM | 18598 | O | HOH W | 65 | | | 3.529 | 1.00 3 | | | ō |
| 25 | ATOM | 18601 | 0 | HOH W | 66 | 33.822 -13 | | 5.347 | 1.00 | | | Ö |
| | MOTA | 18604 | 0 | HOH W | 67 | , | .483 -1 | | 1.00 5 | | | ō |
| | ATOM | 18607 | 0 | HOH W | 68 | 32.094 8 | .727 3 | 34.971 | 1.00 5 | | | ō |
| | MOTA | 18610 | 0 | HOH W | 69 | 22.667 29 | .780 3 | 32.323 | 1.00 5 | 51.06 | | 0 |
| | MOTA | 18613 | 0 | HOH W | 70 | | | 7.793 | 1.00 € | 65.33 | | 0 |
| 30 | MOTA | 18616 | 0 | HOH W | 71 | | | 5.075 | 1.00 6 | | | 0 |
| | MOTA | 18619 | 0 | HOH W | 72 | | | 6.403 | 1.00 5 | | | 0 |
| | ATOM | 18622 | 0 | HOH W | 73 | | .846 -1 | | 1.00 5 | | | 0 |
| | ATOM ATOM | 18625 | 0 | HOH W | 74 | | | 1.975 | 1.00 4 | | | 0 |
| 35 | ATOM | 18628 18631 | 0 | HOH W | 75 76 | | | 4.503 | 1.00 6 | | | 0 |
| ېر | MOTA | 18634 | o | HOH W | 77 | -5.681 42 25.415 -23 | | 4.382 | 1.00 4 | | | 0 |
| • | ATOM | 18637 | Ö | HOH W | 78 | | | 1.860 0.338 | 1.00 3 | | | 0 |
| | ATOM | 18640 | ŏ | HOH W | 79 | | | 8.733 | 1.00 6 | | | 0 |
| | ATOM | 18643 | 0 | HOH W | 80 | | | 2.207 | 1.00 6 | | | .0 |
| 40 | ATOM | 18646 | o ĺ | HOH W | 81 | | | 9.686 | 1.00 5 | | | ō |
| | ATOM | 18649 | 0 | HOH W | 82 | | | 1.382 | 1.00 5 | | | ō |
| | ATOM | 18652 | 0. | нон w | 83 | 15.150 -3 | .137 -2 | | 1.00 5 | | | ō |
| | ATOM | 18655 | O | HOH W | 84 | 48.107 19 | .301 3 | 5.815 | 1.00 8 | 32.63 | | 0 |
| 45 | ATOM | 18658 | О | HOH W | 85 | | .678 1 | 6.423 | 1.00 5 | 57.12 | | 0 |
| 45 | ATOM | 18661 | 0 | HOH W | 86 | | | 7.628 | 1.00 € | | | 0 |
| | ATOM | 18664 | 0 | HOH W | 87 | | | 5.713 | 1,.00 6 | | | 0 |
| • | ATOM | 18667 | 0 | HOH W | 88 | 42.110 -10 | | 7.097 | 1.00 5 | | | О |
| | ATOM | 18670 18673 | 0 | HOH W | 89 | 27.827 -20 | | 8.513 | 1.00 4 | | | 0 |
| 50 | ATOM | 18676 | 0 | HOH W | 90 91 | | | 3.072 | 1.00 5 | | | 0 |
| 50 | ATOM | 18679 | Ö | HOH W | 92 | | | 0.780 | 1.00 5 | | | 0 |
| | ATOM | 18682 | ŏ | HOH W | 93 | | | 1.010 3.290 | 1.00 5 | | | 0 |
| ~~ | ATOM | 18685 | o. | HOH W | 94 | | | 9.374 | 1.00 4 | | | 0 |
| | ATOM | 18688 | Ō | HOH W | 95 | | .087 -19 | | 1.00 7 | | | 0 |
| 55 | ATOM | 18691 | 0 | HOH W | . 96 | | | 8.870 | 1.00 5 | | • | 0 |
| | ATOM | 18694 | 0 | HOH W | 97 | | | 1.202 | 1.00 4 | | | ŏ |
| • | ATOM | 18697 · | 0 | HOH W | 98 | | | 2.655 | 1.00 6 | | | ő |
| | ATOM | 18700 | 0 | HOH W | 99 | 15.664 -12 | | 2.110 | 1.00 5 | | | ŏ |
| C C | ATOM | 18703 | 0 | HOH W | | | | 0.533 | 1.00 4 | | | ŏ |
| 60 | ATOM | 18706 | 0 | HOH W | | | | 4.727 | 1.00 6 | | | ō |
| | ATOM | 18709 | 0 | HOH W | 102 | 46,723 -8 | .667 10 | 6.202 | 1.00 6 | | | O |
| | | | | | | | | | | | | |

| | | | | | | | | • | | |
|-----|--------------|----------------|-----|------------------------|-----------------|------------------|------------------|--------------------------|---|----|
| 5 | ATOM | 18712 | 0 | HOH W 103 | 41.497 | -4.936 | 5.247 | 1.00 35.19 | | 0 |
| | ATOM | 18715 | 0 | HOH W 104 | | -10.122 | | 1.00 39.62 | | ŏ |
| | ATOM | 18718 | 0 | HOH W 105 | 27.866 | 33.167 | 19.639 | 1.00 47.41 | | ō |
| | ATOM | 18721 | 0 | HOH W 106 | 51.713 | 4.314 | 11.942 | 1.00 66.19 | | 0 |
| | ATOM | 18724 | O | HOH W 107 | -0.992 | -3.672 | 8.624 | 1.00 33.89 | | 0 |
| 10 | ATOM | 18727 | 0 | HOH W 108 | 62.335 | 12.316 | 58.893 | 1.00 41.09 | | 0 |
| | ATOM | 18730 | 0 | HOH W 109 | 33.491 | -5.887 | -10.390 | 1.00 41.57 | | 0 |
| | ATOM | 18733 | 0 | HOH W 110 | -5.756 | 74.126 | 24.837 | 1.00 47.70 | | 0 |
| | MOTA | 18736 | 0 | HOH W 111 | 46.526 | 15.070 | 33.144 | 1.00 64.45 | | 0 |
| | ATOM | 18739 | О | HOH W 112 | 18.516 | 31.491 | 45.131 | 1.00 66.88 | | 0 |
| 15 | ATOM | 18742 | 0 | HOH W 113 | 7.469 | 52.148 | 17.072 | 1.00 52.60 | | 0 |
| - | MOTA | 18745 | 0 | HOH W 114 | 9.252 | 52.803 | 15.021 | 1.00 51.30 | | 0 |
| | MOTA | 18748 | Ο. | HOH W 115 | 36.282 | 18.066 | 45.395 | 1.00 47.63 | | 0 |
| | MOTA | 18751 | 0 | HOH W 116 | 17.694 | -5.596 | 0.263 | 1.00 56.44 | | 0. |
| | ATOM | 18754 | 0 | HOH W 117 | 14.604 | -3.959 | 27.588 | 1.00 52.41 | • | 0 |
| 20 | .ATOM | 18757 | 0 | HOH W 118 | 56.706 | 25,271 | 55.385 | 1.00 50.39 | | 0 |
| | MOTA | 18760 | 0 | HOH W 119 | 6.543 | -7.728 | 10.215 | 1.00 54.60 | | 0 |
| | ATOM | 18763 | 0 | HOH W 120 | | -20.233 | 10.919 | 1.00 52.16 | | 0 |
| | ATOM | 18766 | 0 | HOH W 121 | -1.214 | | 12.883 | 1.00 46.46 | | 0 |
| 0.5 | ATOM | 18769 | 0 | HOH W 122 | 6.046 | | -13.628 | 1.00 49.67 | | 0 |
| 25 | ATOM | 18772 | 0 | HOH W 123 | 49.689 | 38.586 | 48.909 | 1.00 55.60 | | 0 |
| | ATOM | 18775 | 0 | HOH W 124 | 45.493 | 54.453 | 19.719 | 1.00 56.14 | | 0 |
| | ATOM | 18778 | 0 | HOH W 125 | 53.857 | -1.594 | 17.970 | 1.00 47.50 | | 0 |
| | ATOM | 18781 | 0 | HOH W 126 | 37.535 | 64.000 | 25.273 | 1.00 57.85 | | 0 |
| 20 | ATOM | 18784 | O, | HOH W 127 | 13.976 | 22.044 | 60.248 | 1.00 40.96 | | 0 |
| 30 | ATOM | 18787 | 0 | HOH W 128 | 23.599 | 74.068 | 17.026 | 1.00 75.23 | | 0 |
| - | MOTA | 18790 | 0 | HOH W 129 | 18.700 | 59.069 | 48.419 | 1.00 50.89 | • | 0 |
| | ATOM | 18793 | . 0 | HOH W 130 | 37.126 | | | 1.00 45.81 | | 0 |
| | ATOM ATOM | 18796 18799 | Ò | HOH W 131 | 35.158 | -8.435 | | 1.00 49.91 | | 0 |
| 35 | ATOM | 18802 | 0 | HOH W 132 HOH W 133 | 7.279 38.706 | 46.170 45.973 | 47.118 60.559 | 1.00 67.83 | | 0 |
| | ATOM | 18805 | Ö | HOH W 134 | 3.810 | 8.884 | 19.812 | 1.00 62.46 1.00 56.91 | | 0 |
| | ATOM | 18808 | Ö | HOH W 135 | 30.111 | 19.847 | 28.143 | 1.00 50.91 | | 0 |
| | ATOM | 18811 | ŏ | HOH W 136 | | -24.638 | 9.123 | 1.00 52.08 | | Ö |
| | ATOM | 18814 | ō | HOH W 137 | 44.787 | 29.869 | 37.519 | 1.00 57.52 | • | ő |
| 40 | ATOM | 18817 | 0 | HOH W 138 | 16.457 | 45.882 | 14.500 | 1.00 50.23 | | Ö. |
| * | MOTA | 18820 | 0 | HOH W 139 | 6.610 | -9.081 | 1.907 | 1.00 66.14 | | ō |
| • | ATOM | 18823 | 0 | HOH W 140 | 30,624 | 17.120 | 56.530 | 1.00 43.89 | | O |
| | ATOM | 18826 | 0 | HOH W 141 | 24.663 | 54.575 | 7.459 | 1.00 75.45 | | O |
| | ATOM | 18829 | 0 | HOH W 142 | 3.291 | 53.721 | 16.115 | 1.00 52.15 | | 0 |
| 45 | ATOM | 18832 | 0 | HOH W 143 | 17.798 | 44.614 | 43.412 | 1.00 35.28 | | 0 |
| | MOTA | 18835 | 0 | HOH W 144 | -3.893 | 63.767 | 39.732 | 1.00 57.61 | | 0 |
| | MOTA | 18838 | 0 | HOH W 145 | 26.346 | -12.103 | -11.462 | 1.00 51.74 | | 0 |
| | ATOM | 18841 | 0 | HOH W 146 | 25.178 | 37.664 | 46.309 | 1.00 42.85 | | 0 |
| | MOTA | 18844 | 0 | HOH W 147 | 10.226 | 70.895 | 7.418 | 1.00 23.44 | | 0 |
| 50 | ATOM | 18847 | 0 | HOH W 148 | 47.426 | -13.956 | 31.608 | 1.00 57.62 | | 0 |
| | MOTA | 18850 | 0 | HOH W 149 | 42.632 | 40.326 | 64.290 | 1.00 46.68 | | 0 |
| | ATOM | 18853 | 0 | HOH W 150 | 47.965 | 16.027 | 69.814 | 1.00 52.99 | | Ο |
| | ATOM | 18856 | 0 | HOH W 151 | 35.258 | 17.505 | 50.695 | 1.00 37.18 | • | 0 |
| | ATOM | 18859 | 0 | HOH W 152 | 42.765 | 25.171 | 73.864 | 1.00 45.61 | | 0 |
| 55 | ATOM | 18862 | 0 | HOH W 153 | 17.682 | 37.118 | 60.178 | 1.00 48.19 | | 0 |
| | ATOM | 18865 | 0 | HOH W 154 | | 51.651 | 20.340 | 1.00 59.26 | | 0 |
| | ATOM | 18868 | 0 | HOH W 155 | 18.284 | | -22.455 | 1.00 66.44 | | 0 |
| | ATOM | 18871 | 0 | HOH W 156 | 48.174 | 37.200 | 72.008 | 1.00 51.47 | | 0 |
| 60 | ATOM | 18874 | 0 | HOH W 157 | 8.994 | 39.168 | 22.488 | 1.00 59.94 | | 0 |
| 60 | ATOM | 18877 | 0 | HOH W 158 | 38.685 | 8.951 | 71.019 | 1.00 53.48 | | 0 |
| | ATOM | 18880 | 0 | HOH W 159 | 43.966 | 16.431 | 65.023 | 1.00 57.15 | | 0 |
| | | | | | | | | • | | |

| | | - | | | | | | | | |
|----|------|-------|----|------------|-----|--------|---------|--------|------------|-----|
| 5 | ATOM | 18883 | Ο. | HOH W | 160 | 45.628 | 3.345 | 77.459 | 1.00 52.32 | 0 |
| _ | MOTA | 18886 | 0 | HOH W | 161 | 49.305 | 24.574 | 45.364 | 1.00 73.80 | 0 |
| | ATOM | 18889 | 0 | HOH W | 162 | 23.302 | 22.739 | 1.013 | 1.00 64.58 | 0 |
| | MOTA | 18892 | 0 | HOH W | 163 | 4.901 | 31.457 | 31.801 | 1.00 63.61 | 0 |
| | ATOM | 18895 | 0 | HOH W | 164 | 35.668 | 9.733 | 38.971 | 1.00 57.20 | 0 |
| 10 | ATOM | 18898 | 0 | HOH W | 165 | 50.588 | 20.385 | 73.103 | 1.00 65.81 | 0 |
| | ATOM | 18901 | 0 | - 'HOH W : | 166 | 27.437 | 13.505 | 15.130 | 1.00 54.05 | 0 |
| | ATOM | 18904 | 0 | HOH W | 167 | 18.140 | 44.428 | 69.479 | 1.00 60.04 | 0 |
| | ATOM | 18907 | 0 | HOH W | 168 | 20.428 | 61.835 | 21.571 | 1.00 50.20 | 0 |
| | ATOM | 18910 | 0 | HOH W | | 16.346 | 20.786 | 61.900 | 1.00 68,58 | . 0 |
| 15 | ATOM | 18913 | 0 | HOH W | 170 | 10.022 | -16.733 | -3.299 | 1.00 45.71 | 0 |
| 10 | ATOM | 18916 | o | HOH W | 171 | 52.508 | 6.294 | 75.257 | 1.00 53.77 | 0 |
| • | ATOM | 18919 | 0 | HOH W | 172 | 58.749 | 6.101 | 66.320 | 1.00 46.84 | 0 |
| | ATOM | 18922 | 0 | нон w | 173 | 28.460 | -0.709 | 0.570 | 1.00 49.98 | 0 |
| - | ATOM | 18925 | 0 | HOH W | 174 | 10.291 | 60.292 | 8.525 | 1.00 55.76 | 0 |
| 20 | ATOM | 18928 | 0 | HOH W | | 4.095 | 2.945 | 15.154 | 1.00 58.94 | . 0 |
| | ATOM | 18931 | 0 | нон w | 176 | 7.244 | -13.384 | -5.254 | 1.00 48.74 | 0 |
| | MOTA | 18934 | 0 | HOH W | 177 | 32.377 | -16.618 | -4.059 | 1.00 44.28 | 0 |
| | ATOM | 18937 | 0 | HOH W | 178 | 47.649 | 0.734 | 67.335 | 1.00 49.13 | 0 |
| | ATOM | 18940 | 0 | HOH W | | 12.789 | 47.261 | 47.980 | 1.00 63.48 | 0 |
| 25 | ATOM | 18943 | 0 | HOH W | 180 | 5.446 | -15.480 | -4.436 | 1.00 57.50 | 0 |
| | ATOM | 18946 | Ó | W HOH | 181 | 9.087 | 37.020 | 24.095 | 1.00 67.94 | 0 |
| | ATOM | 18949 | Ō | HOH W | | 20.864 | -8.162 | 29.795 | 1.00 49.49 | 0 |
| | ATOM | 18952 | 0 | HOH W | 183 | 43.991 | -1.427 | 62.252 | 1.00 55.02 | 0 |
| | | | | | | | | | | |

* * *

Having thus described in detail preferred embodiments of the present invention, it is to be understood that the invention defined by the appended claims is not to be limited by particular details set forth in the above description as many apparent variations thereof are possible without departing from the spirit or scope thereof.

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WHAT IS CLAIMED IS:

A catalytic domain of BACE or a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or an apo-BACE crystal or an apo-BACE crystal that can be soaked to give complexes and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme or between about pH 5.6 and about pH 5.8 and/or a BACE crystal having a space group of C2 and/or a BACE crystal having cell dimensions of a= 236.63Å or 236.63Å ± standard deviation (0.2Å) or 236.63Å \pm 3.0Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or $105.02\text{Å} \pm 3.0\text{Å}$, and c= 62.59Å or $62.59\text{Å} \pm \text{standard deviation}$ (0.2Å) or 62.59Å \pm 3.0Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm 3.0Å, b= 107.4Å \pm standard deviation (0.2Å) or $107.4\text{Å} \pm 3.0\text{Å}$, and c= 60.4Å or $60.4\text{Å} \pm \text{standard deviation}$ (0.2Å) or $60.4\text{\AA} \pm 3.0\text{\AA}$ and $\beta=101.89^{\circ}$ or $101.89^{\circ} \pm$ standard deviation (0.2°) or between 101° and 108° and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing; and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P2₁ form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand; and/or a BACE crystal having a resolution better than 3 Å; and/or a BACE crystal having the structure defined by the co-ordinates of Table 5.

- 2. A BACE crystal having the structure defined by the co-ordinates of Table 5.
- 3. An apo-BACE crystal grown at or near the physiological pH of the enzyme.
- 4. An apo-BACE crystal or an apo-BACE crystal that can be soaked to give complexes.
- 5. A crystalline form of BACE or a functional portion thereof having crystals that are grown at or near the physiological pH of the enzyme.
- 6. The crystalline form of BACE or functional portion thereof of claim 6 wherein the crystals are grown at a pH between about pH 5.6 and about pH 5.8

7. A crystalline form of BACE or a functional portion thereof having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) 236.63Å \pm 3.0Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or 105.02Å \pm 3.0Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm 3.0Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm 3.0Å, b= 107.4Å or 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm 3.0Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm 3.0Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P2₁ together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P2₁ form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand.

- 8. A crystalline form of BACE or a functional portion thereof that has an active site containing one or more ligands other than the natural substrate or the substrate that occurs naturally or physiologically within the active site.
- 9. A method for ligand screening or identification comprising exposing the BACE crystals of any one of claims 2-8 to one or more test samples, and determining whether a ligand-BACE complex is formed.
- 10. The method of claim 9 wherein the BACE protein or functional portion thereof is exposed to the test samples by co-crystallizing the BACE protein or functional portion thereof in the presence of the one or more test samples.
- 11. The method of claim 9 wherein the BACE of claims 2-8 is soaked in a solution of one or more test samples
- 12. A computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE or a functional portion thereof:

comprising using a programmed computer comprising a processor, a data storage system, an input device, and an output device, the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the

atoms in the BACE catalytic domain, optionally with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system; (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said data set; (d) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said data set and (e) outputting to said output device the selected chemical structures having a portion similar to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits BACE; or,

comprising: providing the structure of BACE as defined by the co-ordinates of Table 5, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the structure of the BACE of Table 5; or,

comprising: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"), providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the selected co-ordinates of BACE; or,

comprising: providing the co-ordinates of at least a sub-domain of BACE, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the sub-domain of BACE;

said method optionally further comprising: obtaining or synthesizing the chemical structure or candidate modulator and contacting the chemical structure or candidate modulator with BACE to determine the ability of the chemical structure or candidate to interact with BACE; or obtaining or synthesizing the chemical structure or candidate modulator and forming a complex of BACE and said chemical structure or candidate modulator, and analyzing the complex to determine the ability of said chemical structure or candidate modulator to interact with BACE.

13. A compound having a chemical structure selected using the methods of claims 9-12, said compound being a modulator of BACE

- 14. A BACE protein or functional portion thereof comprising amino acid sequences of the catalytic domain that crystallize to the crystalline structure of claim 7, or to a structure that mimics that crystalline structure.
- 15. A BACE protein or functional portion thereof which, when compared to wild-type BACE or BACE of Genbank accession P56817 has one or more mutations or truncations to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals.
- 16. The BACE protein or functional portion thereof of claim 15, which when compared with Genbank accession P56817 has one or more of: a mutation at amino acid ("aa") 153, a mutation at aa 172, a mutation at aa 223, a mutation at aa 354, and one or more truncations.
- 17. The BACE protein or functional portion thereof of claim 16 wherein each of the mutations is asparagine to glutamine.
- 18. The BACE protein or functional portion thereof of claim 16 wherein the truncation results in a BACE extending from Thr 22 to Ser 453, with reference to Genbank Accession P56817.
- 19. The BACE protein or functional portion thereof of claim 16 wherein all of the mutations are present and each is asparagine to glutamine and there is a truncation resulting in a BACE extending from Thr 22 to Ser 453, with reference to Genbank Accession P56817.
- 20. The BACE protein or functional portion thereof of any one of claims 14-19 further including any one or more of: a tag to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium; and a tag to allow differentiation of species arising from incomplete pro-peptide cleavage.
- 21. The BACE protein or functional portion thereof of claim 20 wherein the tag to facilitate purification is a HIS tag, the non-BACE signal sequence is a baculovirus signal sequence, and the tag to allow differentiation of species is a FLAG tag.
- 22. The BACE protein or functional portion thereof of claim 21 wherein all of the tag to facilitate purification, the non-BACE signal sequence and the tag to allow differentiation are present.

23. A BACE protein or functional portion thereof containing any one or more of: a tag to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium; and a tag to allow differentiation of species arising from incomplete pro-peptide cleavage.

- 24. The BACE protein or functional portion thereof of claim 23 wherein the tag to facilitate purification is a HIS tag, the non-BACE signal sequence is a baculovirus signal sequence, and the tag to allow differentiation of species is a FLAG tag.
- 25. The BACE protein or functional portion thereof of claim 24 wherein all of the tag to facilitate purification, the non-BACE signal sequence and the tag to allow differentiation are present.
- 26. An isolated nucleic acid molecule encoding a BACE protein or functional portion thereof of any of claims 14-25 or a functional portion thereof.
- 27. The isolated nucleic acid molecule of claim 26 that has a reduced GC content via silent mutations from nucleotide sequences derived from wild-type BACE that would also encode the BACE protein.
 - 28. A vector or cell comprising or expressing the nucleic acid molecule of claim 26.
 - 29. A vector or cell comprising or expressing the nucleic acid molecule of claim 27.
- 30. The vector or cell of claim 28 which is a viral vector or a bacterial vector or a mammalian cell or a DNA plasmid.
- 31. The vector or cell of claim 29 which is a viral vector or a bacterial vector or a mammalian cell or a DNA plasmid.
- 32. The vector or cell of claims 30 or 31 which is a baculovirus vector or an insect cell.
- 33. The vector or cell of claim 26 further including a nucleic acid molecule encoding an enhancer that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein.
- 34. The vector or cell of claim 27 further including a nucleic acid molecule encoding an enhancer that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein.
- 35. The vector or cell of claims 33 or 34 wherein the enhancer is a prohormone convertase.

36. The vector or cell of claim 35 wherein the prohormone convertase is furin.

- 37. A vector or cell comprising a nucleic acid molecule encoding a BACE protein or functional portion thereof and a nucleic acid molecule encoding an enhancer that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein.
 - 38. The vector or cell of claim 37 wherein the enhancer is a prohormone convertase.
- 39. A kit for producing the vector or cell of claim 37 containing separately packaged nucleic acid molecules comprising (i) a BACE-protein encoding nucleic acid molecule and (ii) a nucleic acid molecule encoding the enhancer.
- 40. A method for obtaining a BACE protein comprising expressing a nucleic acid molecule according to any of claims 26 or 27 or the nucleic acid molecule of the vector or cell of any of claims 28 to 34 or 37.
- 41. A method for obtaining a BACE protein comprising expressing the nucleic acid molecule of the vector or cell of claim comprising expressing in a vector or cell the nucleic acid molecules of the kit of claim 39.
- 42. A method for crystallizing a BACE protein or functional portion thereof comprising dissolving a BACE protein according to any one of claims 14-25 in a suitable solvent and crystallizing the same either in the presence or absence of an inhibitor; wherein said method optionally further includes producing the BACE recombinantly or by expression thereof by a vector, recovering the BACE so produced, and growing crystals from the recovered BACE.
 - 43. The method of claim 42 wherein the inhibitor is OM99-2.
- 44. A method for determining the crystal structure of a BACE protein or functional portion thereof comprising obtaining crystals of a BACE protein according to any one of claims 14-25 and obtaining an x-ray diffraction pattern thereof.
- 45. A method for ligand screening and design or identification comprising exposing the BACE crystals of a BACE protein or functional portion thereof to one or more test samples, and determining whether a ligand-BACE complex is formed; wherein the BACE or functional portion thereof has an unoccupied active site and is as claimed in any one of claims 5-8.

46. The method of claim 45 wherein the BACE is exposed to the test samples by either co-crystallizing the BACE or functional portion thereof in the presence of the one or more test samples or soaking the BACE or a functional portion thereof in a solution of one or more test samples.

47. A computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE or a functional portion thereof:

comprising using a programmed computer comprising a processor, a data storage system, an input device, and an output device, the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the atoms in the BACE catalytic domain or functional portion thereof of any one of claims 5-8, optionally with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system; (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said data set; (d) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said data set and (e) outputting to said output device the selected chemical structures having a portion similar to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits BACE; or,

comprising: providing the structure of BACE as defined by the co-ordinates of Table 5, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the structure of the BACE of Table 5; or,

comprising: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"), providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the selected co-ordinates of BACE; or,

comprising: providing the co-ordinates of at least a sub-domain of BACE, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the sub-domain of BACE;

said method optionally further comprising: obtaining or synthesizing the chemical structure or candidate modulator and contacting the chemical structure or candidate modulator with BACE

to determine the ability of the chemical structure or candidate to interact with BACE; or obtaining or synthesizing the chemical structure or candidate modulator and forming a complex of BACE and said chemical structure or candidate modulator, and analyzing the complex to determine the ability of said chemical structure or candidate modulator to interact with BACE.

- 48. A ligand identified in any of the methods of claims 45-47.
- 49. An assay comprising a BACE protein or functional portion thereof of any one of claims 14-25, and means to determine whether a compound is a modulator of BACE.
- 50. An antibody elicited by a BACE protein or functional portion thereof of any one of claims 14-25.
- 51. An inhibitor of a BACE protein or functional portion thereof of any one of claims 14-25.
 - 52. A composition comprising the inhibitor of claim 51.
 - 53. A composition comprising the ligand of claim 48.
 - 54. A composition comprising the ligand of claim 13.
 - 55. A composition comprising a product from the assay of claim 49.
- 56. A method for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof comprising administering an inhibitor of a BACE protein or functional portion thereof as claimed in claim 51.
- 57. A method for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof comprising administering a ligand of claim 13.
- 58. A method for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof comprising administering a ligand of claim 48.
- 59. A BACE which comprises an amino acid sequence of SEQ ID NO: 5 or an amino acid sequence having greater than 98.8% identity with SEQ ID NO:5.
 - 60. The BACE of claim 59 having the amino acid sequence of SEQ ID NO:5.
 - 61. A nucleic acid molecule encoding the BACE of claim 59 or 60.
- 62. An isolated nucleic acid molecule comprising a sequence of SEQ ID NO: 4 or 10 or a sequence having greater than 95.6% identity with SEQ ID NO: 4 or 10.
- 63. The isolated nucleic acid molecule of claim 62 having the sequence of SEQ ID NO:4.

64. The isolated nucleic acid molecule of claim 63 having the sequence of SEQ ID NO:10.

- 65. A vector or cell comprising the isolated nucleic acid molecule of any one of claims 62-64.
 - 66. The vector or cell of claim 65 which is a baculovirus vector or an insect cell.
 - 67. An inhibitor of the BACE of any one of claims 59 or 60.
 - 68. An antibody elicited by the BACE of any one of claims 59 or 60.
- 69. A method for ligand screening and design or identification comprising exposing the BACE crystals of a BACE protein or functional portion thereof to one or more test samples, and determining whether a ligand-BACE complex is formed; wherein the BACE or functional portion thereof has an unoccupied active site and is as claimed in any one of claims 59 or 60.
- 70. The method of claim 69 wherein the BACE is exposed to the test samples by either co-crystallizing the BACE or functional portion thereof in the presence of the one or more test samples or soaking the BACE or a functional portion thereof in a solution of one or more test samples.
- 71. A computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE or a functional portion thereof:

comprising using a programmed computer comprising a processor, a data storage system, an input device, and an output device, the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the atoms in the BACE catalytic domain or functional portion thereof of any one of claims 59 or 60, optionally with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system; (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said data set; (d) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said data set and (e) outputting to said output device the selected chemical structures having a portion similar to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized

selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits BACE; or,

comprising: providing the structure of BACE as defined by the co-ordinates of Table 5, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the structure of the BACE of Table 5; or,

comprising: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"), providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the selected co-ordinates of BACE; or,

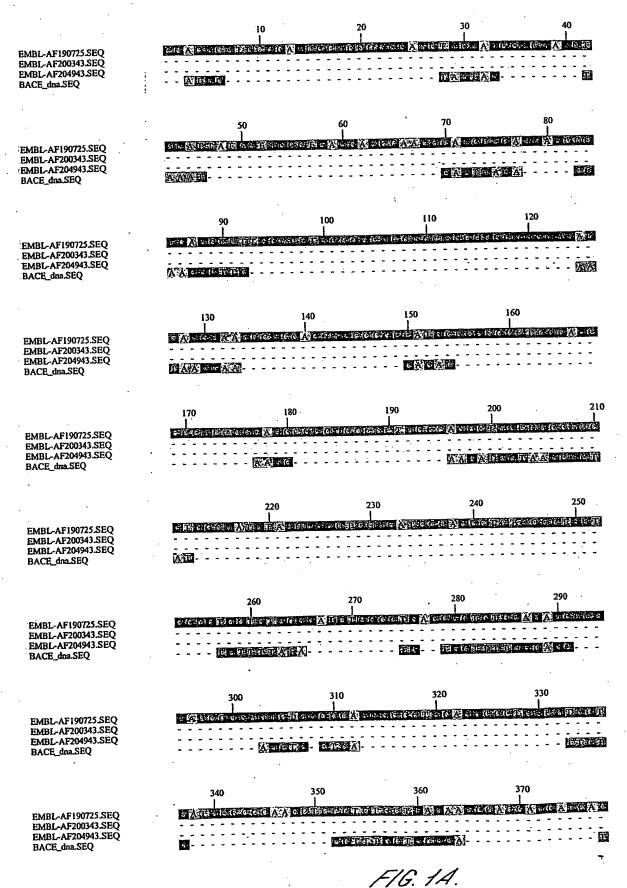
comprising: providing the co-ordinates of at least a sub-domain of BACE, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the sub-domain of BACE;

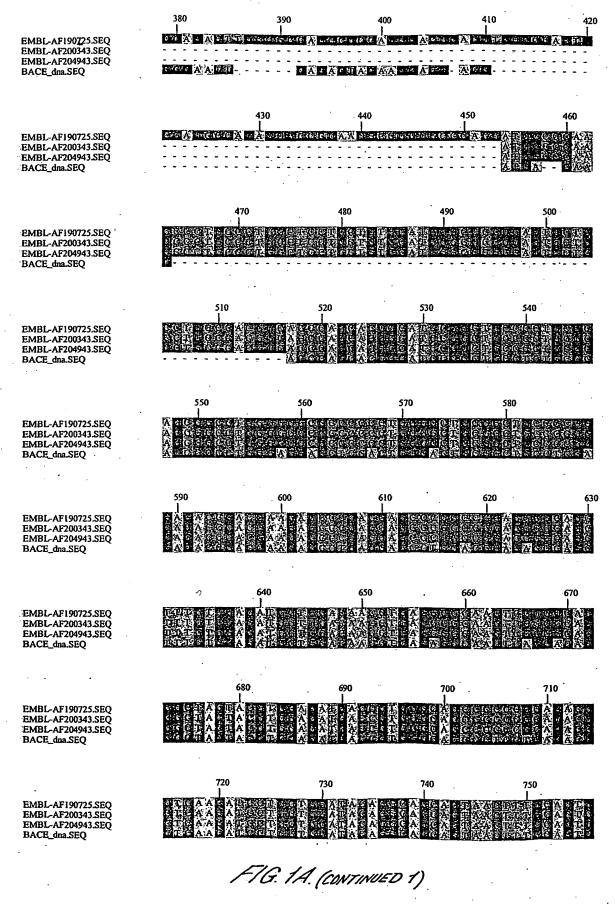
said method optionally further comprising: obtaining or synthesizing the chemical structure or candidate modulator and contacting the chemical structure or candidate modulator with BACE to determine the ability of the chemical structure or candidate to interact with BACE; or obtaining or synthesizing the chemical structure or candidate modulator and forming a complex of BACE and said chemical structure or candidate modulator, and analyzing the complex to determine the ability of said chemical structure or candidate modulator to interact with BACE.

- 72. A ligand identified in any of the methods of claims 68-71.
- 73. An assay comprising a BACE protein or functional portion thereof of any one of claims 58 or 59, and means to determine whether a compound is a modulator of BACE.
 - 74. A composition comprising the inhibitor of claim 67.
 - 75. A composition comprising the ligand of claim 72.
 - 76. A composition comprising a product from the assay of claim 73.
- 77. A method for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof comprising administering an inhibitor of a BACE protein or functional portion thereof as claimed in claim 67.
- 78. A method for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof comprising administering a ligand of claim 72.
- 79. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 51 for preparing a composition or medicament for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof.

80. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 13 for preparing a composition or medicament for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof.

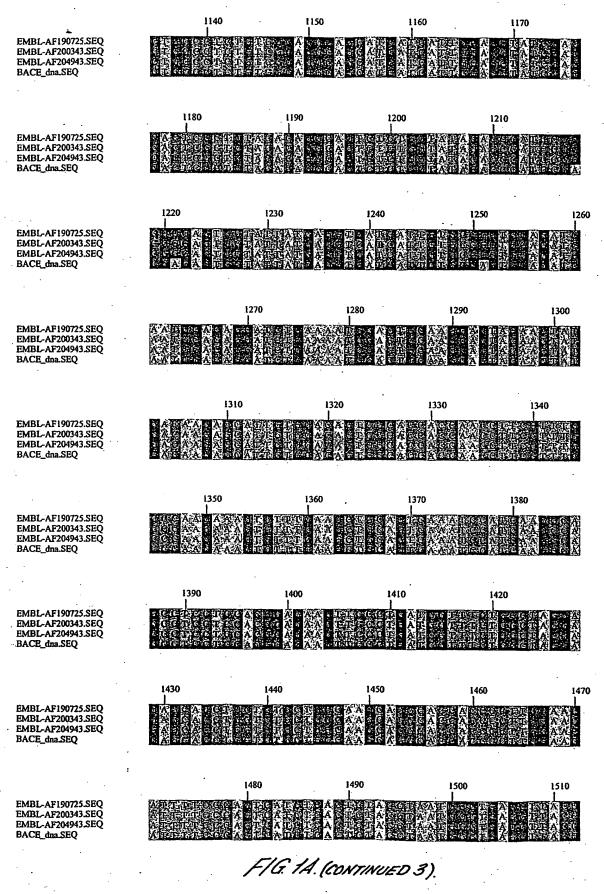
- 81. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 48 for preparing a composition or medicament for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof.
- 82. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 51 for use in therapy.
- 83. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 67 for preparing a composition or medicament for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof.
- 84. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 72 for preparing a composition or medicament for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof.
- 85. A computer system for generating structures or performing rational compound or drug design for BACE or complexes of BACE with a potential modulator, the system containing either: atomic co-ordinate data according to Table 5, said data defining the three-dimensional structure of BACE or at least one sub-domain thereof, or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5.
- 86. A computer readable media with either: atomic co-ordinate data according to Table 5, said data defining the three-dimensional structure of BACE or at least one subdomain thereof, or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5.
- 87. A method of doing business comprising providing to a user the computer system of claim 85 or the computer readable media of claim 83 or the three-dimensional structure of BACE or at least one sub-domain thereof, or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5.

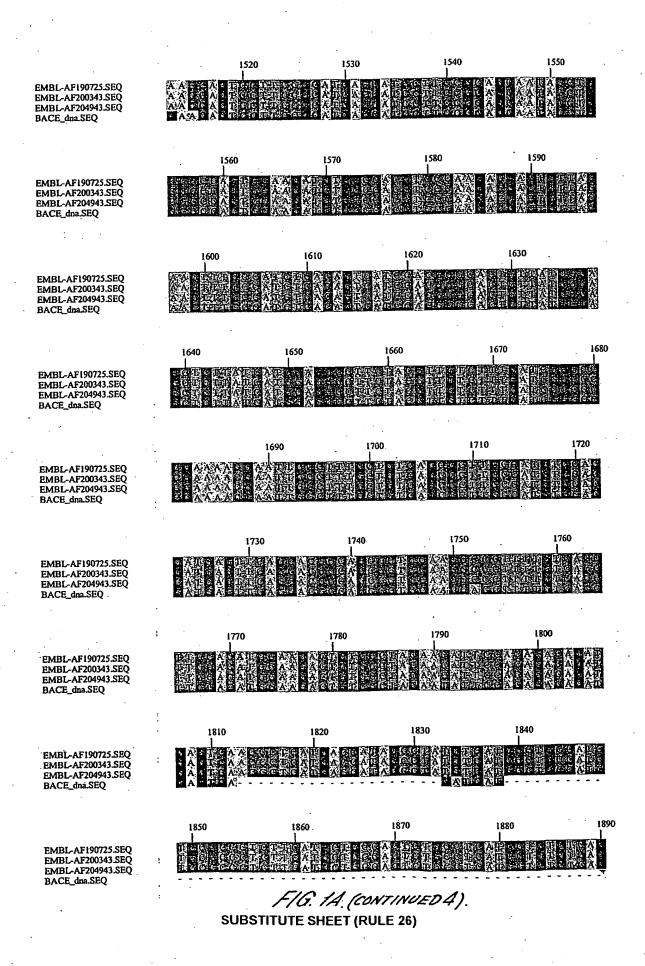


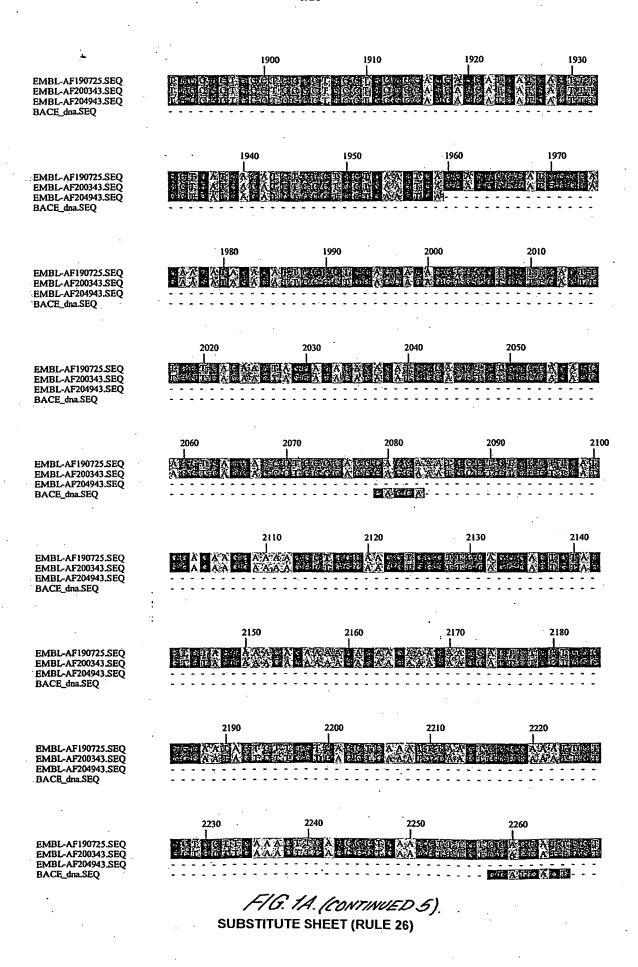


EMBL-AF190725.SEQ EMBL-AF200343.SEQ EMBL-AF204943.SEQ BACE_dna.SEQ

F/G. 1A. (CONTINUED 2).







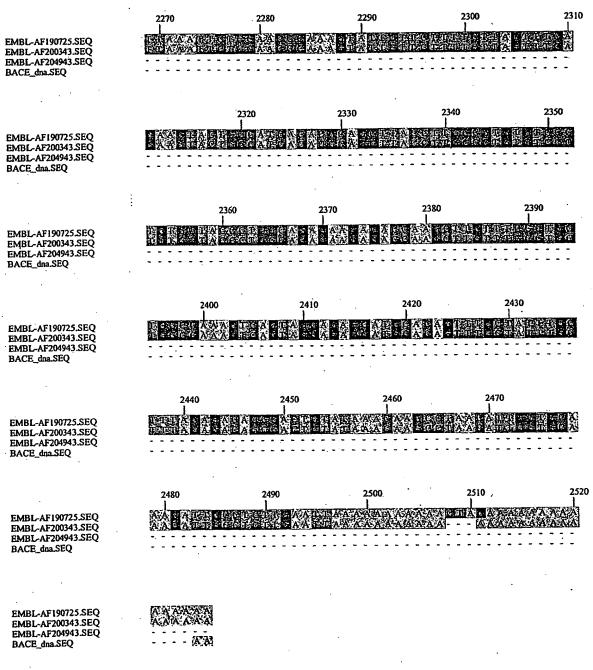


FIG. 1A. (CONTINUED 6).

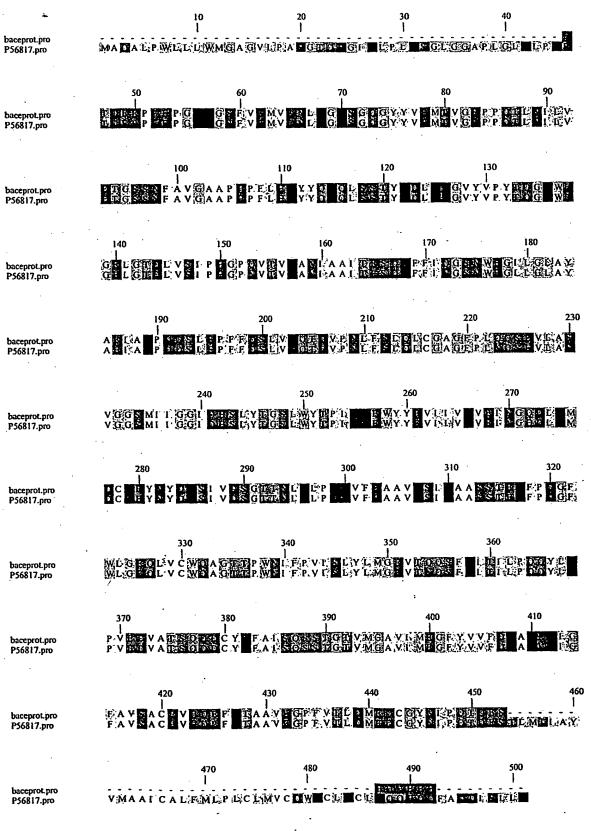


FIG. 18.

| ETDEEPEEPG | RRGSFVEMVD | NLRGKSGQGY | YVEMTVGSPP | QTLNILVDTG | SSNFAVGAAP | 60 |
|------------|------------|------------|------------|------------|------------|-----|
| HPFLHRYYOR | QLSSTYRDLR | KGVYVPYTQG | KWEGELGTDL | VSIPHGPQVT | VRANIAAITE | 120 |
| SDKFFIQGSN | WEGILGLAYA | EIARPDDSLE | PFFDSLVKQT | HVPNLFSLQL | CGAGFPLQQS | 180 |
| | | TGSLWYTPIR | | | | 240 |
| | | VKSIKAASST | | | | 300 |
| LYLMGEVTQQ | SFRITILPQQ | YLRPVEDVAT | SQDDCYKFAI | SQSSTGTVMG | AVIMEGFYVV | 360 |
| PUDADKRICE | AVSACHVHDE | FRTAAVEGPF | VTLDMEDCGY | NIPOTDESHH | HHHH | 414 |

FIG. 2A

GCTTTTGGCAGCAGCTGCTCATTCTGCCTTTGCTGCGGATCCGAATTCAGACTACAAGGACGACGATGACAAGACCCAGC ACGGATCCGCTGCCTCTGCGCAGCGGCCTGGGAGGAGCTCCACTGGGACTGCGCTGCCTCGAGAGACCGACGAAGAG GGAGATGACCGTGGCCAGCCCTCCTCAGACGCTCAACATCCTGGTGGATACAGGCAGCAGTAACTTTGCAGTGGTGCTG CACCACACCCATTCCTGCATCGCTACTACCAGAGGCAGCTGTCCAGCACATACCGAGACCTACGGAAGGGTGTGTATGTG CCCTACACCCAGGCCAAGTGGGAAGGAGGAGCTGGCACCGACCTGGTAAGCATCCCCCATGGACCTCAAGTCACTGTGCG TGCCAACATTGCTGCCATCACTGAATCAGACAAGTTCTTCATCCAAGGCTCCAACTGGGAAGGCATCCTGGGGCTGGCCT TGGAGGTATCGACCACTCGCTGTACACAGGCAGTCTCTGGTATACACCCATCCGAGGAGGTGGTATTATGAGGTGATCA TTGTGCGAGTGGAGATCAATGGACAGGATCTGAAAATGGACTGCAAGGAGTACAACTATGACAAGAGCATTGTGGACAGT GGCACCACCAACCTTCGTTTGCCCAAGAAAGTGTTTGAAGCTGCAGTCAAATCCATCAAGGCAGCCTCCTCCACGGAGAA GTTCCCTGATGGTTTCTGGCTAGGAGAGCAGCTGGTGTGCTGGCAAGCAGGCACCACCCCTTGGAACATTTTCCCAGTCA TCTCACTCTACCTAATGGGTGAGGTTACCCAACAGTCCTTCCGCATCACCATCCTTCCGCAGCAATACCTGCGGCCAGTG GAAGATGTGGCCACGTCCCAAGACGACTGTTACAAGTTTGCCATCTCACAGTCATCCACGGCACTGTTATGGGAGCTGT TATCATGGAGGGCTTCTACGTTGTCTTTGATCGGGCCCGAAAACGAATTGGCTTTGCTGTCAGCGCTTGCCATGTGCACG ATGAGTTCAGGACGGCAGCGGTGGAAGGACCTTTTGTCACCTTGGACATGGAAGACTGTGGCTACAATATTCCACAGACA GATGAGTCACATCATCACCACCATCACTAA

FIG. 2B.

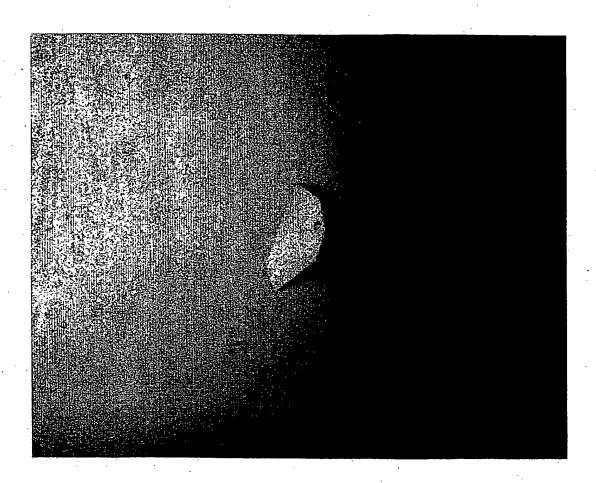


FIG. 3A.

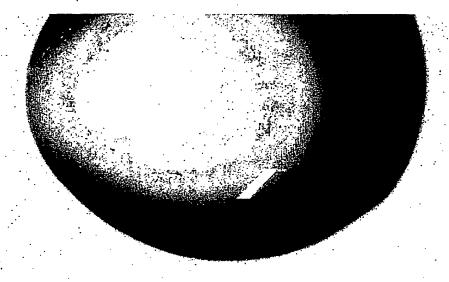


FIG. 3B.

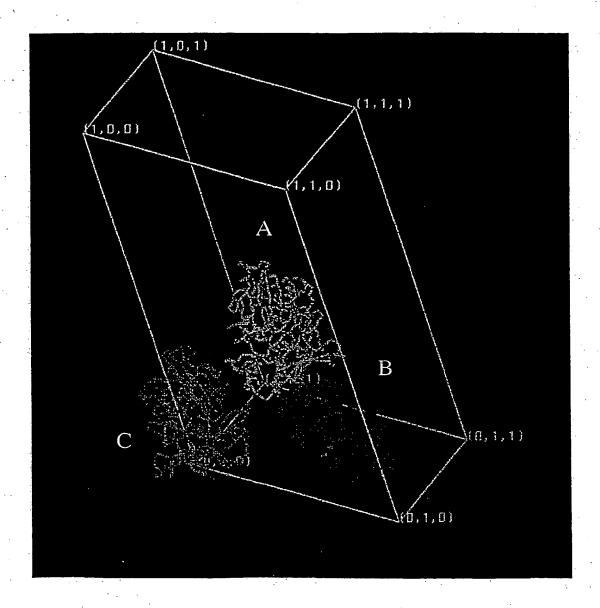


FIG. 4A.

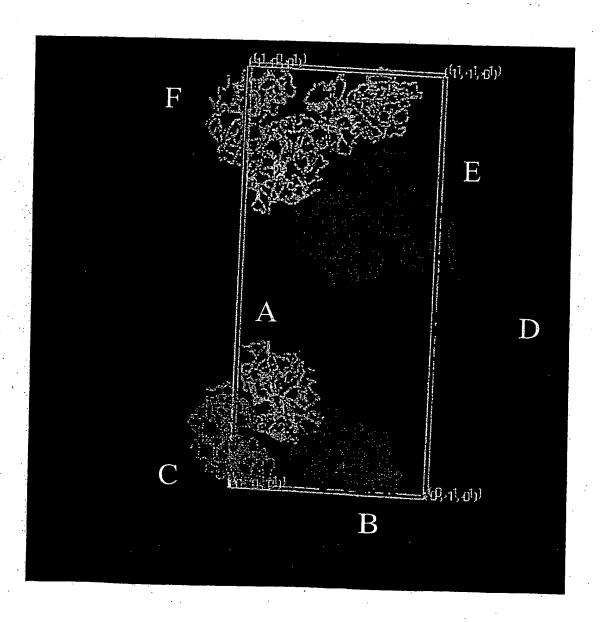
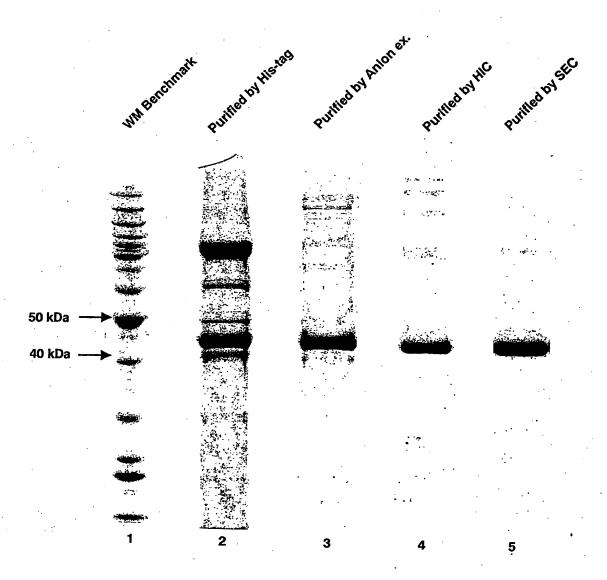
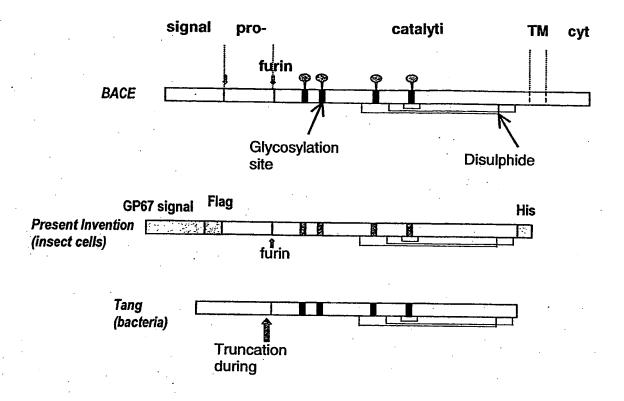


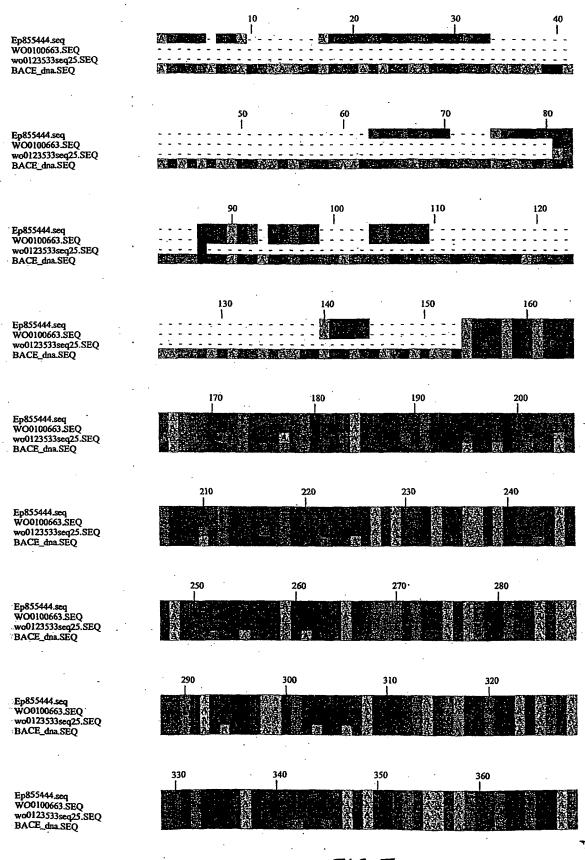
FIG. 4B.



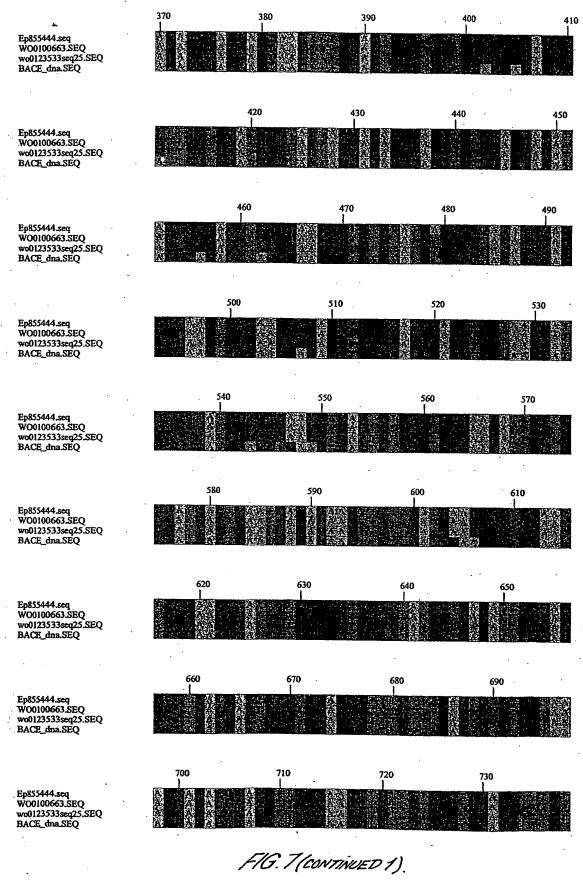
F/G. 5.



F1G. 6.



F/G. 7.
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FIG. 7 (CONTINUED 2).
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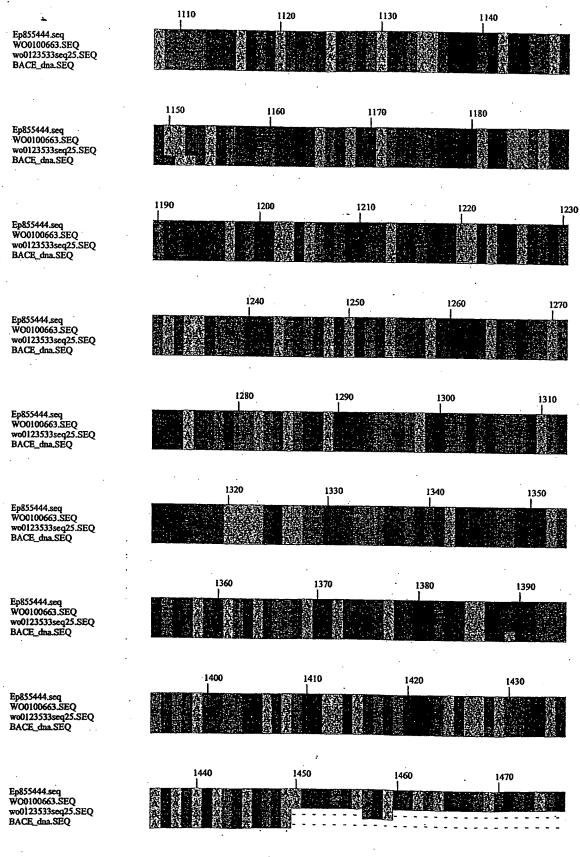


FIG. T(CONTINUED 3).
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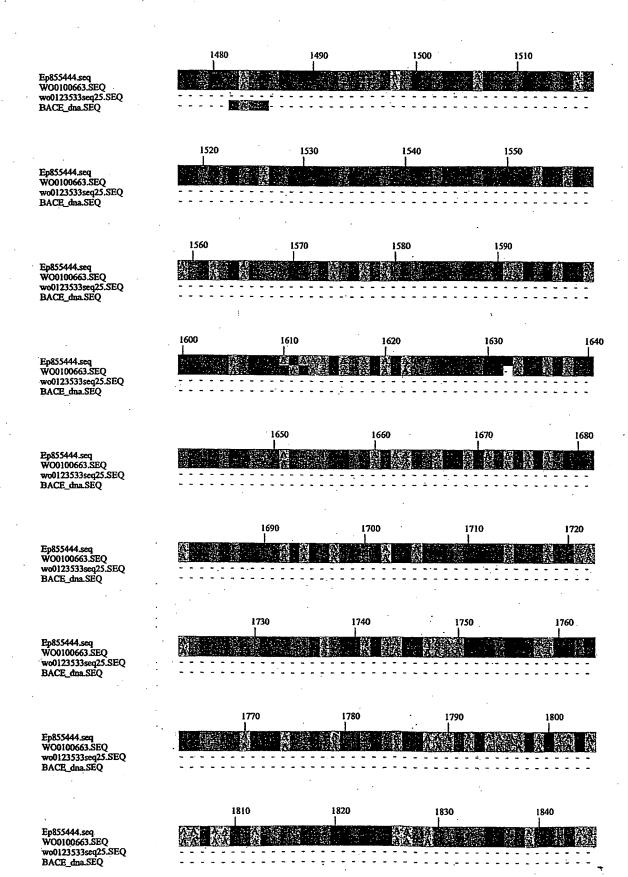
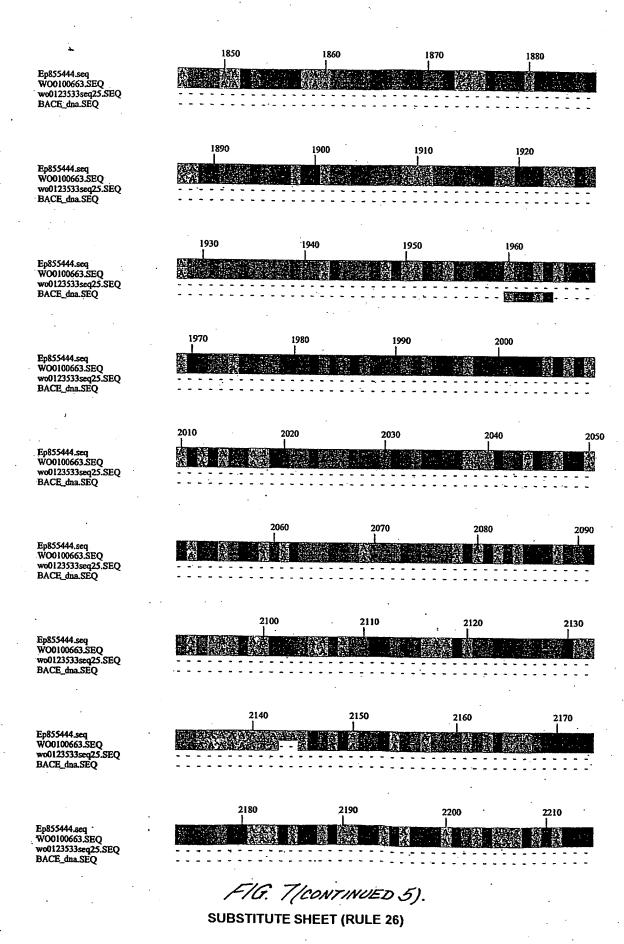
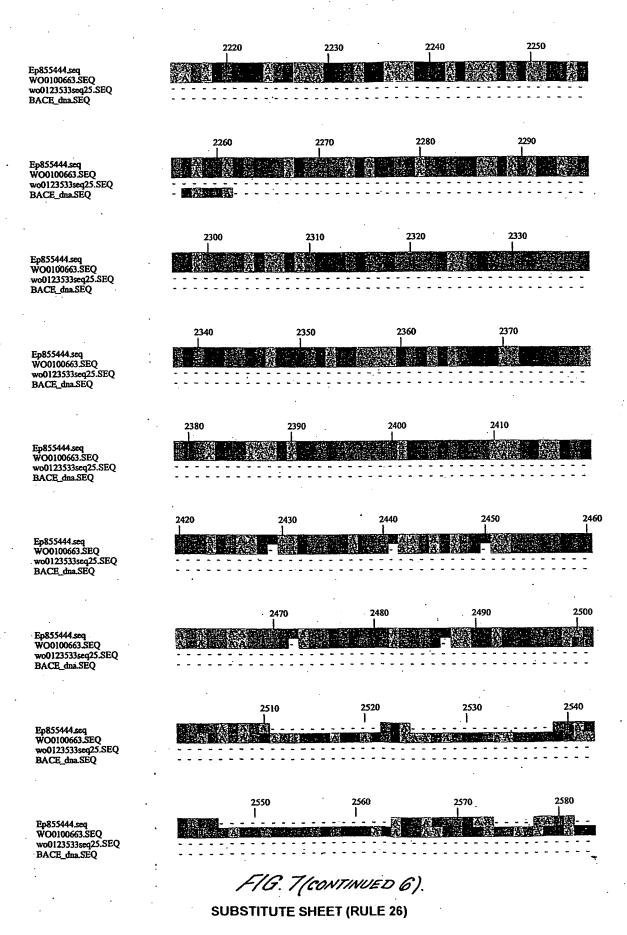
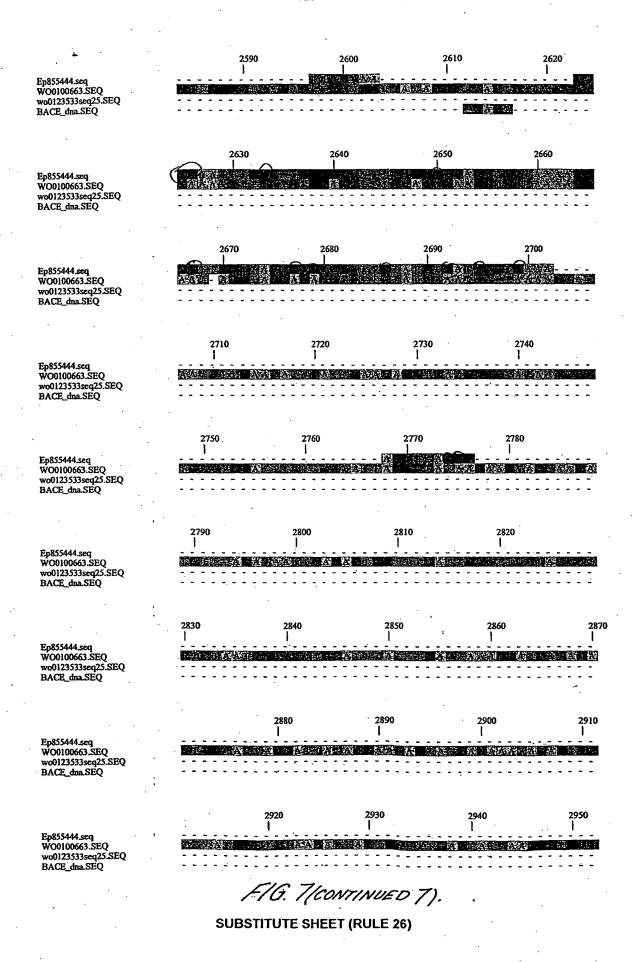


FIG. T/CONTINUED 4).







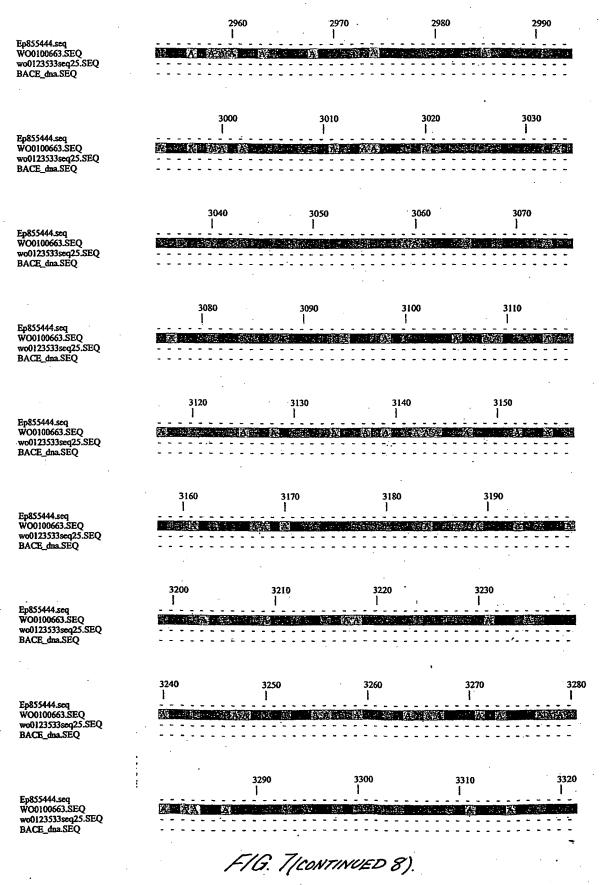
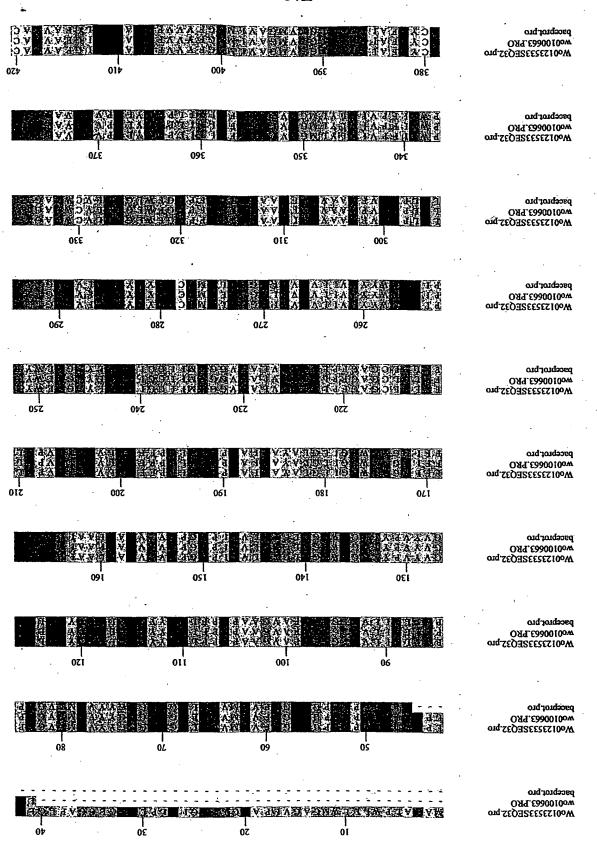


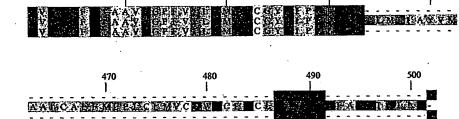
FIG. T(CONTINUED 9).

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89/



Wo0123533SEQ32.pro wo0100663.PRO baceprot.pro



Wo0123533SEQ32.pro wo0100663.PRO baceprot.pro

FIG. 8 (CONTINUED).